

TI A **statistical** approach to **catalyst** development. I. The effect of
 process variables on the vapor-phase oxidation of naphthalene
 AU Franklin, N. L.; Pinchbeck, P. H.; Popper, F.
 CS Univ. Leeds, UK
 SO Transactions of the Institution of Chemical Engineers (1956), 34, 280-93
 CODEN: TICEAH; ISSN: 0371-7496
 DT Journal
 LA Unavailable
 AB The results of a **statistical** approach to the detn. of the optimum
 conditions for the vapor-phase oxidation of C₁₀H₈ (I) with air and a
 moderated V2O₅ **catalyst** are reported in detail. The expts. were
 conducted in a 1-in. diam. fluidized bed reactor. A fluidized bed was
 used because the reaction is highly exothermic and maintenance of a
 uniform reaction **temp.** is easier in a fluidized bed. The app. consisted
 of an air preheater passing air at approx. 100° over the feed
 delivery tube, picking up the I as vapor. The air-I mixt. was further
 preheated before entering the reactor. The fluidized bed was supported on
 a stainless-steel sintered disk and surrounded by a batch of heat-transfer
 salt. The oxidation products included o-C₆H₄(CO)₂O (II), maleic
 anhydride, 1,4-naphthoquinone, CO, and CO₂. The variables studied
 included the air-I ratio, **contact** time, and bed **temp.** The max. yield
 of II at any **temp.** is approx. const. over the range studied. At lower
temps., longer reaction times and greater air concns. are required to
 reach high yields, and at const. **temp.**, longer **contact** times are
 required with lower air-I ratios. The results indicate that the reaction
 rate is proportional to the O concn. and that the rate of O adsorption on
 the **catalyst** surface is controlling. Regression equations are developed
 to define the yield contours for all of the products as a function of
contact time and air-I ratio over the range investigated.

=> log y

STN INTERNATIONAL LOGOFF AT 12:40:30 ON 19 FEB 2004

CS Inst. Neftekhim. Sint., Moscow, USSR
SO Koks i Khimiya (1982), (6), 25-7
CODEN: KOKKAI; ISSN: 0023-2815

DT Journal
LA Russian

AB The optimum **temp.** and **space velocity** in the hydrocracking of the dild. naphthalene [91-20-3] fraction of coal tar with coke gas-derived H₂ on an Al-Co-Mo **catalyst** were detd. from **statistically** designed expts.. The high-grade naphthalene prepd. under optimum conditions in 105% yield was suitable for producing phthalic anhydride [85-44-9] and S-free benzene [71-43-2].

L8 ANSWER 9 OF 17 CA COPYRIGHT 2004 ACS on STN

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AN 96:106782 CA

TI Optimum conditions for the alkylation of isobutane by propylene on a polyfunctional **catalyst**

AU Areshidze, Kh. I.; Chkheidze, G. S.; Mortikov, E. S.; Zen'kovskii, S. M.; Pogorelov, A. G.; Yanchevskaya, T. I.

CS Inst. Org. Khim., Kazan, USSR
SO Neftekhimiya (1981), 21(5), 669-73
CODEN: NEFTAH; ISSN: 0028-2421

DT Journal
LA Russian

AB A **statistically**-designed exptl. plan was used to det. the optimum **temp.** (x₁), **space velocity** (x₂), and isobutane [75-28-5] to propylene (I) [115-07-1] ratio (x₃) in the syntheses of isooctanes modeling **catalytic** alkylation in the manuf. of gasoline components. The best combination of I conversion (98.3%) and selectivity of isooctane formation (76.8%) were obtained at x₁ = 130°, x₂ = 0.5h⁻¹, and x₃ = 18.1.

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[ZwbqZXNPeGZX1aYsqg5ZJFchyvV@I sWFUCwGl7F9yJ8HSaTY@E@p3E7KCP7lhtZwEM@uKrJldBVyRTuQqjkFHKqtplAIFjRKeoeM8i@YbjJtq0zzk7@TWmnhQ25pToWHW7DfK690@7bzEFCeToGLHtIt8](https://chemport.cas.org/cgi-bin/cp_sdcgi?ZwbqZXNPeGZX1aYsqg5ZJFchyvV@I sWFUCwGl7F9yJ8HSaTY@E@p3E7KCP7lhtZwEM@uKrJldBVyRTuQqjkFHKqtplAIFjRKeoeM8i@YbjJtq0zzk7@TWmnhQ25pToWHW7DfK690@7bzEFCeToGLHtIt8)>

AN 88:89219 CA

TI Disproportionation of toluene: **process optimization** by **statistical design** of experiments

AU Rawat, D. S.; Bawa, J. S.; Shanker, Uma; Dabral, R. P.; Bhattacharyya, K. K.

CS Indian Inst. Pet., Dehra Dun, India
SO Indian Journal of Technology (1977), 15(3), 114-18
CODEN: IJOTA8; ISSN: 0019-5669

DT Journal
LA English

AB The disproportionation of toluene to benzene and xylenes over a zeolite **catalyst** was planned **statistically** (orthogonal central composite design) in the **temp.** range 440-510, 10-50 kg/cm² **pressure**, **space velocity** (WHSV) 0.58-3.41 and H to toluene molar ratio 4-11. The conversion of toluene was correlated with these **process variables** by a 2nd degree polynomial, the unknown coeffs. of which were evaluated by the least squares method. The values of optimum conversion at different values of WHSV predicted from the correlation were confirmed by subsequent expts. The model generated contours of conversion which indicate operating variables for a desired level of conversion.

L8 ANSWER 17 OF 17 CA COPYRIGHT 2004 ACS on STN

Full Text <[https://chemport.cas.org/cgi-bin/cp_sdcgi?](https://chemport.cas.org/cgi-bin/cp_sdcgi?rw9qAXNPeGZX1aYlqg5ZJFchyvV@I sWFUCwGl7F9yJ8HSaUY@E@p3E7KCP7lhtZwEM@uKrJldBVyRTuQqskFHKqtplAIFjRKeceM8i@YbjJtq0zzk7@TWmnhQ25pToWHW7DfK690@V zlFoeToCLxt8t4)

[rw9qAXNPeGZX1aYlqg5ZJFchyvV@I sWFUCwGl7F9yJ8HSaUY@E@p3E7KCP7lhtZwEM@uKrJldBVyRTuQqskFHKqtplAIFjRKeceM8i@YbjJtq0zzk7@TWmnhQ25pToWHW7DfK690@V zlFoeToCLxt8t4](https://chemport.cas.org/cgi-bin/cp_sdcgi?rw9qAXNPeGZX1aYlqg5ZJFchyvV@I sWFUCwGl7F9yJ8HSaUY@E@p3E7KCP7lhtZwEM@uKrJldBVyRTuQqskFHKqtplAIFjRKeceM8i@YbjJtq0zzk7@TWmnhQ25pToWHW7DfK690@V zlFoeToCLxt8t4)>

AN 51:56666 CA

OREF 51:10452e-h

- L14 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Ethylene oligomerization with Ni(MeCN)₆(BF₄)₂ in homogeneous phase, immobilized in ionic liquids or heterogenized in zeolite
 AU Oberson de Souza, Michele; de Souza, Roberto F.
 SO Current Topics in Catalysis (2002), 3, 267-273
 CODEN: CTCTFP

AB The oligomerization of alkenes has been performed with Ni(MeCN)₆(BF₄)₂ associated with AlEt₂Cl or AlEt₃ as cocatalysts under different catalytic conditions: in homogeneous phase, under biphasic conditions (immobilized in ionic liqs.) or heterogenized in zeolite. Ni(MeCN)₆(BF₄)₂ in homogeneous phase shows high activity (TOF = 2451 h⁻¹) and selectivity to C₄ products (97%) with 30% of 1-butene under mild reaction conditions (10 bar, 50°C). Ni(MeCN)₆(BF₄)₂ dissolved in 1-methyl-3-butyl-imidazolium chloride/AlEt₂Cl/AlEt₂Cl₂ ionic liqs. catalyzes ethylene dimerization with a selectivity that can attain 83% in 1-butene and Ni(MeCN)₆(BF₄)₂ immobilized in zeolite (NaX) exhibit selectivities in 1-butene of 78 %. The behavior of the same complex [Ni(MeCN)₆(BF₄)₂] acting under these different catalytic reaction conditions (homogeneous, biphasic and heterogeneous) is compared and discussed. The active species and the mechanism for ethylene dimerization are proposed and discussed based on concerned characterization studies.

- L14 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Fischer-Tropsch synthesis: induction and steady-state activity of high-alpha potassium promoted iron catalysts

AU Luo, Mingsheng; O'Brien, Robert J.; Bao, Shiqi; Davis, Burtron H.

SO Applied Catalysis, A: General (2003), 239(1-2), 111-120

CODEN: ACAGE4; ISSN: 0926-860X

AB Iron Fischer-Tropsch synthesis (FTS) catalysts with different potassium loadings showed different induction periods during which the conversion increased from a low initial level to a peak value before declining to attain a lower stable activity at the same reaction conditions. A lower K loading produced a slightly higher peak conversion and a shorter induction period. Although, the induction period and the peak conversion were slightly dependent on the K loading for the iron catalyst, the stabilized conversions and the stabilization periods were independent of potassium content. The C₂-C₄ olefin to paraffin ratio of the gaseous products and the CO₂ selectivity did not change significantly as the potassium content increased from 5 to 10%. An increase in reaction temperature produced a new induction period and a

higher conversion than was obtained before the reaction temperature was increased. The H₂/CO ratio also had an important influence on FTS conversions. Increasing the H₂/CO ratio in the feed gas lowered the H₂ use. A higher H₂/CO ratio feedstock gas produced lower FTS catalyst activity compared to a low H₂/CO ratio gas.

- L14 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Dimerization of 1-butene catalyzed by zirconium complexes

AU Zhang, Yu-liang; Li, Bao-jun; He, Ren

SO Dalian Ligong Daxue Xuebao (2001), 41(4), 416-420

CODEN: DLXUEJ; ISSN: 1000-8608

AB Dimerization of 1-butene was catalyzed by the complexes ZrCl₄, Zr(CCl₃CO₂)₄, Zr(OEt)₂Cl₂ with Et₂AlCl. The effects of different reaction conditions on the 1-butene dimerization have been studied, and the structures of main products also tested. In the same reaction condition, the order of the 1-butene conversion of the catalysts is Zr(CCl₃CO₂)₄ > ZrCl₄ > Zr(OEt)₂Cl₂. Under the optimal reaction conditions, the conversion of the catalyst Zr(CCl₃CO₂)₄-Et₂AlCl-Ph₃P is 95.1% with selectivity of 85.4% for dimerization. C₆ olefins have been found in the dimerization products, so the metal carbon mechanism for 1-butene oligomerization by zirconium complexes is proposed.

- L14 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI A novel cross-aldol condensation for preparation of hydroxypivaldehyde using simple phase-transfer catalysts

IN Mahmud, Meftahuddin; Vishwakarma, Lal C.; Faizi, Ahmad Kamal

SO Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

AB A method for the condensation of aldehydes is disclosed in which an aldehyde containing an <SYM97>-hydrogen atom and having the formula R1CHO [R1 = C1-12 alkyl, C1-14 aralkyl] is combined with a phase-transfer catalyst R₄X⁺ Y⁻ [R = same or different alkyl

or aralkyl group; X = N or P; Y = any atom or group of atoms, particularly OH, making a basic counter anion] under reaction conditions to give a mixture comprising an aldol, an unsatd.

aldehyde derived by dehydration of the aldol, or both. Alternatively, an aldehyde R1CHO reacts with a second aldehyde R2CHO [R₂ = H, C1-12 alkyl,

C1-14 aralkyl] and a catalyst, to form the crossed aldol, the unsatd.

aldehyde derived by dehydration of the crossed aldol, or both. The formed aldol or aldehyde may be separated from the reaction mixture and recovered or treated as desired, or the reaction mixture may be further treated (e.g., by hydrogenation), to produce a desired product mixture (e.g., containing

neopentyl

glycol). For example, condensation of isobutyraldehyde with aqueous formaldehyde under stirring in the presence of slowly added PhCH₂N⁺Me₃

OH-

catalyst at 21-22° (caution: exothermic) gave hydroxypivaldehyde

plus a desired byproduct, neopentyl glycol (2-5%), with 100%

selectivity, and with 95.17% conversion of

isobutyraldehyde. The product is extractable with EtOAc or iso-BuAc, with the catalyst remaining in the aqueous phase for recycle. The reaction is well reproducible, including scale-ups.

- L14 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Process for the preparation of olefin oxides

IN Paparatto, Giuseppe; Forlin, Anna; Tegen, Paolo

SO Eur. Pat. Appl., 10 pp.

CODEN: EPXXDW

AB A process in continuous is described for the preparation of oxides of olefins by the direct epoxidn. of an olefin with H₂O₂, or compds. capable of producing H₂O₂ under the reaction conditions, in a solvent medium, in the presence of a catalytic system consisting of a zeolite containing titanium and a nitrogenated organic base having formula

NRR1R₂, wherein R, R₁, and R₂ = the same or different,

can be H, a C1-10 alkyl, a -COR₃ where R₃ is a C1-10 alkyl, or a

-CR₄R₅(CH₂)_nOH, wherein n = 1-10 and R₄, R₅ = H or a C1-10 alkyl, on the condition that R, R₁, and R₂ are not contemporaneously H. Thus, 1970 g/h methanol-water solution, 230 g/h aqueous H₂O₂ (35% by weight), 12 bar propylene, and

100 g/h water containing 0.23% ethanolamine were fed to a reactor in the presence of 40 g TS 1 and 760 g methanol-water solution for 6 h at 60° to give a propylene oxide with H₂O₂ conversion 94% and propylene oxide selectivity 97.5%.

- L14 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Oxidative coupling of methane as a method for natural gas chemical utilization

AU Filkova, D.; Petrov, L.

SO Bulgarian Chemistry and Industry (1998), 69(34), 107-112

CODEN: BCINF9; ISSN: 1311-1663

AB Source. A review, with 54 refs. Natural gas is considered a promising alternative to the crude oil both as a raw material for valuable chemical substances and as an energy. The trends in searching for highly active and selective catalysts for oxidative coupling of methane (OCM) are discussed. Three groups of catalysts for OCM are discussed: solid solns. based on rare earth metal oxides, solid solns. containing elements of variable oxidation state, and perovskites with different content of substituting cations within the same crystal phase. It is generally accepted that methane activation occurs on the catalyst surface where Me radicals couple to form ethane. The radicals released into the gas phase lead to a pool of radicals that set up a complex reaction network. The relative contribution of homogeneous and heterogeneous reaction steps is under discussion but most studies point out that the suppression of homogeneous reactions improves the selectivity. It is obvious that no single and simple mechanisms can apply to different catalysts and reaction conditions.

- L14 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Stability test of MgO/BaCO₃ catalyst for oxidative coupling of methane in fixed-bed reactor

AU Ding, Yan; Ding, Xuejia; Wang, Xiaolai; Da, Jianwen; Shen, Shikong

SO Shiyu Huangong (1996), 25(4), 241-248

CODEN: SHHUE8; ISSN: 1000-8144

AB Two types of circular and tubular thin layer fixed bed reactors were used to facilitate the reaction heat transfer for the stability tests of MgO/BaCO₃ catalyst. The catalyst was very stable during the tests. In the tubular fixed-bed, with CH₄:O₂:H₂O = 5:1:7.8 and CH₄ GHSV of 5000 h⁻¹,

- a CH₄ conversion of 25%, a C₂ selectivity of 65% and a C₂ yield of 16.2% were achieved. In the circular fixed-bed, with CH₄:O₂:H₂O = 5:1:2.3 and CH₄ GHSV of 5700 h⁻¹, a CH₄ conversion of 26%, a C₂ selectivity of 67.5% and a C₂ yield of 17.3% were achieved. Pure oxygen as oxidant and water vapor as diluent facilitated the seps. of the products. Water vapor was beneficial to the transfer of reaction heat and lowered the temperature difference in the catalyst bed. The structure of the catalysts were almost the same before and after the reaction. The effects of different reaction conditions, such as the residence time of CH₄, temperature of reactor wall, water vapor content, were also investigated.

L14 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Selectivity control by oxygen pressure in methane oxidation over phosphate catalysts

AU Sinev, M. Yu.; Setiadi, S.; Otsuka, K.

SO Studies in Surface Science and Catalysis (1994), 82(New Developments in Selective Oxidation II), 357-65

CODEN: SSCTDM; ISSN: 0167-2991

AB Oxidative transformations of methane are studied over a series of phosphate catalysts. Over Zr-P and Zn-P catalysts the shifts from formaldehyde to C₂-hydrocarbons were observed at oxygen concentration and temperature

variations indicating their formation via common intermediate, likely CH₃-radicals. Different products selectivities over different catalysts in the same reaction conditions demonstrate the participation of the surface in products formation.

L14 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Selectivity control by oxygen pressure in methane oxidation over phosphate catalysts

AU Sinev, Mikhail Yu.; Setiadi, S.; Otsuka, Kiyoshi

SO Mendeleev Communications (1993), (1), 10-11

CODEN: MENCEX; ISSN: 0959-9436

AB Selectivity shifts from formaldehyde to ethane with oxygen pressure and temperature variation in methane oxidation over phosphate catalysts are evidence for the existence of mutual intermediate and different product selectivities over different catalysts under the same reaction conditions, indicating the participation of the surface in formaldehyde formation.

L14 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Base- and acid-catalysed cyclization of diketones over ZSM-5

AU Dessau, R. M.

SO Zeolites (1990), 10(3), 205-6

CODEN: ZEOLD3; ISSN: 0144-2449

AB The acid-catalyzed cyclization of acetonylacetone at 350° over a 300:1 silicon/aluminum HZSM-5 yielded >97% 2,5-dimethylfuran. In contrast, the calcined, excess sodium-containing, basic form of this same catalyst produced an entirely different cyclization product, 3-methyl-2-cyclopenten-1-one, in greater than 89% yield under identical reaction conditions. This base-catalyzed cyclization reaction can be used diagnostically to determine the presence of basic sites in zeolitic catalysts.

L14 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Tin analogs of the vinyllogous Reformatsky reaction. Regio- and stereochemical considerations

AU Fan, Ru Lin; Hudlicky, Tomas

SO Tetrahedron Letters (1989), 30(41), 5533-6

CODEN: TELEAY; ISSN: 0040-4039

GI

AB Condensation reaction of Bu₃SnCH₂CR:CHCO₂Et (I, R = Me, OMe) with benzaldehyde and cyclohexanone were studied under different reaction conditions. The regio- and stereochem. profiles were determined in an effort to control the course of dienolate addns. to carbonyl compds. under acid-catalyzed conditions. Thus, BF₃·Et₂O catalyzed reaction of I (R = Me) with PhCHO in CH₂Cl₂ at -78° in 2 h gave 91% threo-PhCH(OH)CH(CO₂Et)CHMe:CH₂ (II), whereas the same reaction at -78° for 2 h followed by 14°

at 5.5 h gave 10% II along with 90% phenylpranone III in total 85% yield.

L14 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Reaction of chlorobenzene, carbon monoxide and benzene under high pressure

AU Goswami, A. K.; Murty, K. R.; Palit, S. K.

SO Indian Journal of Technology (1976), 14(6), 2947

CODEN: IJOTA8; ISSN: 0019-5669

AB Reaction of PhCl with CO and C₆H₆ at high pressure over a CaO/Na aluminosilicate catalyst gave BzH 1.17, BzCl 5.52, and phthalic acid 2.38%, based on PhCl input and under the same set of optimum reaction conditions, whereas under a different set of optimum reaction conditions, the yields of BzOH and Ph₂CO were 75.42 and 4.84%, resp.

L14 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Activation of catalysts by <SYM103>-rays for the manufacture of gas

AU Macak, Jiri; Tymlova, Jindriska

SO Sbomik Vysoke Skoly Chemicko-Technologicke v Praze, D: Technologie Paliv

(1967), No. 14, 73-85

CODEN: SVCTA6; ISSN: 0554-9736

AB In a continuous tubular laboratory reactor the activity of industrial and laboratory

prepared catalysts of the Ni-Al₂O₃ type for the reaction of cyclohexane with water vapor was studied. Prior to testing, the catalysts were subjected to preliminary irradiation with <SYM103>-rays (60Co) of different intensity and dosage, and the results obtained were compared with those obtained under the same reaction conditions on nonirradiated catalysts. The activity of the industrial catalysts was pos. affected only with a dose >(1-2) + 107 rads, while with the dose of 4 + 107 rads it was already possible to achieve, in dependence on the quality of the catalyst, a 1.3-2.3 fold increase in the yield of the gaseous products (reaction temperature 720°, atmospheric pressure). The catalyst prepared in the

laboratory by impregnation of a pure corundum carrier contained different amts.

of Ni. In testing the nonirradiated catalysts, the dependence of the gas yield on the active component content showed a certain maximum in the concentration range 3-8% of Ni with the catalyst used; this, however, was lowered

as a result of irradiation. For this purpose, two sources of <SYM103>-rays of different intensity were used. With a lower dosing intensity under otherwise equal conditions of irradiation and testing, the gas yield decreased in the whole concentration range of the active component, with a higher

dosing intensity this decrease was not so pronounced. The leveling of the maximum was more pronounced with the higher dosing intensity. The results obtained were used also for evaluating the operating mode of a tubular continuous reactor.

L14 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Long chain vinyl ethers and esters, their polymers and copolymers. II.

Preparation, purification, and Characterization of some long chain vinyl esters

AU Chatterjee, P. C.; Dakshinamurty, H.; Aggarwal, J. S.

SO Indian Journal of Technology (1966), 4(6), 1735

CODEN: IJOTA8; ISSN: 0019-5669

AB cf. CA 62, 8993f. By replacing 100% H₂SO₄ catalyst in the conventional vinyl interchange process by 40% HF, higher yields (70-75%) of vinyl esters of fatty acids of different chain lengths and unsatns. (lauric, palmitic, stearic, oleic, linoleic, and linolenic) and of mixed fatty acids from safflower and linseed oils were obtained under the same reaction conditions (acid-vinyl acetate mole ratio, 1:6; refluxing period, 3 hrs.) as in the conventional process which gives much lower yields (30-60%). Replacement of the more expensive vinyl acetate by acetylene, did riot give satisfactory results in respect of both yields of the vinyl esters and simplicity of operation.

L14 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Aromatic hydrocarbons from diarylalkanes

IN Fetterly, Lloyd C.

AB C₂-Alkyl-substituted aromatic hydrocarbons are produced by catalytic cracking of 1,1-diarylalkane hydrocarbons containing 2 aryl substituents on the same C atom of an alkane containing at least 2 C

atoms in the presence of at least 1 mole H/mole hydrocarbon and a composite catalyst of a high-melting inorg. acidic substance and a dehydrogenation catalyst at at least 300°/atmospheric-700 lb./sq. in. Different products can be produced from a single starting material by varying the reaction conditions. Thus, starting with 1,1-dithiolethane, such products as p-ethyltoluene, p-methylstyrene, and 1,1-dithiolethylene can be produced in good yields by suitable adjustment of catalyst, temperature, pressure, and H/hydrocarbon ratio.

L14 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

TI Methylchlorosilanes

IN Sauer, Robert O.

AB A shift of alkyl groups and halogen atoms from one Si atom to another occurs when compds. of the general formulas R_mSiX_{4-m} and R'_nSiX_{4-n} (where

R and R' are lower alkyl radicals, X is halogen, m is 1, 2, or 3, and n is 0, 1, 2, or 3) react with each other at temps. above 250°. An equilibrium relationship is established in which the distribution of the reaction products is in a definite and substantially predictable ratio, depending on the starting materials. The relationship is not in accord with random distribution theory. Redistribution occurs when the 2 alkylhalosilanes are different or when they are the same, as e.g., Me_2SiCl_2 . A side reaction also occurs at temps. of 400° or above, in which dealkylation of the alkylhalosilane takes place with formation of about 10-20% of a reaction product containing a Si-CH₂-Si linkage. Satisfactory reaction conditions vary over wide limits of temperature (250-600°), time, presence of catalyst, and pressure. Superatm. pressures permit lower reaction temps. at slightly longer periods of time with side reactions being minimized. $AlCl_3$ is the only catalyst found which accelerates the reaction. BCl_3 , $ZnCl_2$, $FeCl_3$, and $CuCl_2$ have no perceptible effect on the course of the reaction. Good results are obtained with about 0.5-5% by weight of $AlCl_3$, based on total weight

of silanes employed. At 250-400°, in presence of $AlCl_3$, reaction is complete in 3-20 hrs. Thus, 7.81 moles Me_3SiCl (I) and 20 g. $AlCl_3$ in a steel bomb heated 15.3 hrs. at 300° and 775 lb./sq. in., and the contents, after they had cooled, fractionally distilled yielded Me_2SiCl_2 (II) 0.60 mole, Me_4Si (III) 0.75, and recovered I 5.97 moles. At 450° and 1575 lb./sq. in. with no catalyst, substantially the same results were obtained. II 7.80 moles + $AlCl_3$ 7 hrs. at 350° and 925 lb./sq. in. yielded I 0.85 and $MeSiCl_3$ (IV) 0.84 mole, the remainder being unchanged II. Equimolar quantities of I and IV + $AlCl_3$ in 7 hrs. at 375° gave an equilibrium mixture containing I 10-12, IV 10-12, and II 78-80 mole-%. I 5.18 and $SiCl_4$ (V) 2.58 moles + $AlCl_3$ in 23.5 hrs. at 375° and 1075 lb./sq. in. gave unchanged I 0.55, IV 0.85 mole, and a trace of V; the balance of the product was II. I 3.96, and V 3.93 moles, and $AlCl_3$ heated 7.1 hrs. at 375° and 1290 lb./sq. in. yielded I 0.11, V 0.70, IV 1.91, and II 3.67 moles. IV + $AlCl_3$ in 7 hrs. at 375° and 925 lb./sq. in. gave a trace of V, a small amount of II, and mostly unchanged starting material. II 3.45 and V 3.39 moles heated 17 hrs. at 375° and 900 lb./sq. in. with catalyst yielded a trace of I, II 2.18, IV 1.42, and V 2.24 moles. Raising the temperature to 450°, increased the yield of IV to 3.28 moles. A considerable volume of CH_4 and 123 g. $CH_2(SiCl_3)_2$, b. about 185°, were also obtained. Their formation is attributed to dealkylation of IV at elevated temps. in the presence of $AlCl_3$. Et_2SiCl_2 530 and $AlCl_3$ 10 g. heated 8 hrs. at 300° gave 33 g. $EtSiCl_3$, the balance being unchanged Et_2SiCl_2 containing about 10% Et_3SiCl . Equimolar quantities of Et_2SiCl_2 and V, heated with $AlCl_3$ 7 hrs. at 375° and 1100 lb./sq. in., yielded a small amount of $EtSiCl_3$ as the only product. An equimolar mixture (95.6 g.) of Me_3SiBr and $MeSiBr_3$, heated 6 hrs. at 310-20° with 0.5 g. $AlCl_3$, gave 45.1 g. Me_2SiBr_2 and lesser amts. of starting materials. I heated 7 hrs. at 375° and 1150 lb./sq. in. in the presence of $AlCl_3$ gave small amts. of II, III, and $CH_2(SiClMe_2)_2$, b. about 176°. Equimolar quantities of II and $EtSiCl_3$ heated 5 hrs. in a closed bomb at 375°, $NaCl$ added, and the mixture heated 3.25 hrs. at 225° gave a mixture of $EtSiCl_3$ and $EtMeSiCl_2$, which was converted to the respective EtO compds. on treatment with absolute $EtOH$; $EtMeSi(OEt)_2$, b. 140°, n_D 1.3950, was isolated. In order to establish that $EtMeSiCl_2$ had been obtained, $EtMeSi(OEt)_2$ was treated with PBr_3 to give $EtMeSiBr_2$ b. 139-41°. IV (8.02 moles), heated 7 hrs. at 450° with a catalyst gave V 0.77, II 0.25 mole, a mixture of $CH_2(SiCl_3)_2$ and $Cl_3SiCH_2SiCl_2$, b. 184.3-6.3°, and 5.03 moles unchanged IV. $PhSiCl_3$ 1.87 and I 1.90 mole, heated 4 hrs. at 325° with $AlCl_3$, and the mixture distilled gave I 16, IV 60, II 201, and C_6H_6 28 g. Distillation of the residue yielded a high-boiling mixture, shown by conversion to the corresponding ethoxysilanes, to

contain $PhSiCl_3$ and $MePhSiCl_2$. $PhSiCl_3$ and II yielded a similar mixture which, treated with absolute $EtOH$ and then anhydrous HF , gave $MePhSiF_2$, b.

141-2°. $PhSiCl_3$, and Et_2SiCl_2 (1.99 moles each) heated 7 hrs. at 350° with a catalyst, $NaCl$ added, and the mixture heated 3.5 hrs. at 225° gave V 0.17, C_6H_6 0.73, $EtSiCl_3$ 0.91, Et_2SiCl_2 1.13, $PhSiCl_3$ 0.53 mole, and a high-boiling residue which with absolute $EtOH$ and anhydrous HF yielded $EtPhSiF_2$, b. 163-4°. The dealkylated products, such as $CH_2(SiClMe_2)_2$, are useful as intermediates in the preparation of resins, oils, and synthetic elastomers. 7 references.

L12 ANSWER 1 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Reactivity of triglycerides and fatty acids of rapeseed oil in supercritical alcohols

AU Warabi, Yuichiro; Kusdiana, Dadan; Saka, Shiro

SO Bioresource Technology (2004), 91(3), 283-287

CODEN: BIRTEB; ISSN: 0960-8524

AB A catalyst-free biodiesel production method with supercrit. methanol has been developed that allows a simple process and high yield because of simultaneous transesterification of triglycerides and Me esterification of fatty acids. From these lines of evidence, we expected that similar results would be attained with the use of various alcs. by the supercrit. treatment. However, it still remains unclear which type of reaction, transesterification or alkyl esterification, is faster. This parameter would be important in designing the optimum reaction conditions of the supercrit. alc. method. Therefore, we studied the effect of transesterification of triglycerides and esterification of fatty acids in rapeseed oil. Reaction temperature was set at 300 °C, and methanol, ethanol, 1-propanol, 1-butanol or 1-octanol was used as the reactant. The results showed that transesterification of triglycerides (rapeseed oil) was slower in reaction rates than alkyl esterification of fatty acids for any of the alcs. employed. Furthermore, saturated fatty acids such as palmitic and stearic acids had slightly lower reactivity than that of the unsatd. fatty acids; oleic, linoleic and linolenic.

L12 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Palladium-Catalyzed Carbonylative Annulation of Internal Alkynes:

Synthesis of 3,4-Disubstituted Coumarins

AU Kadnikov, Dmitry V.; Larock, Richard C.

SO Journal of Organic Chemistry (2003), 68(24), 9423-9432

CODEN: JOCEAH; ISSN: 0022-3263

AB The palladium-catalyzed annulation of internal alkynes by o-iodophenols in the presence of CO results in exclusive formation of coumarins. No isomeric chromones have been observed. The best reaction conditions utilize 2-iodophenol, 5 equiv of alkyne, 1 atm of CO, 5 mol % $Pd(OAc)_2$, 2 equiv of pyridine, and 1 equiv of n-Bu₄NCl in DMF at 120

°C. The use of a sterically unhindered pyridine base is essential to achieve high yields. A wide variety of 3,4-disubstituted coumarins containing alkyl, aryl, silyl, alkoxy, acyl, and ester groups have been prepared in moderate to good yields. Mixts. of regioisomers have been obtained when unsym. alkynes are employed. 2-Iodophenols with electron-withdrawing and electron-donating substituents and 3-iodo-2-pyridone are effective in this annulation process. For example, the reaction of 2-iodophenol with (1-butynyl)benzene gave a mixture of 4-ethyl-3-phenyl-2H-1-benzopyran-2-one and 3-ethyl-4-phenyl-2H-1-benzopyran-2-one. The reaction is believed to proceed via (1) oxidative addition of 2-iodophenol to $Pd(0)$, (2) insertion of the alkyne triple bond into the aryl-palladium bond, (3) CO insertion into the resulting vinylic carbon-palladium bond, and (4) nucleophilic attack of the phenolic oxygen on the carbonyl carbon of the acylpalladium complex with simultaneous regeneration of the $Pd(0)$ catalyst. This annulation process is the first example of intermol. insertion of an alkyne occurring in preference to CO insertion.

L12 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Comparing catalytic distillation to separate reaction and distillation for the production of diacetone alcohol

AU Nicol, W.

SO Chemical Engineering Research and Design (2003), 81(A8), 1026-1032

CODEN: CERDEE; ISSN: 0263-8762

AB Diacetone alc. (DAA) is produced via the aldol condensation of acetone. The reaction is severely equilibrium-limited and high conversions of acetone are only possible if the unconverted acetone is separated and recycled. The reaction, separation and recycle can either be done sep. in a reactor-distillation column-recycle process (RDR) or simultaneously in

a catalytic distillation (CD) column. This work compares the sep. process to the simultaneous process. An anion exchange resin was used to catalyze the reaction. Under the studied reaction conditions DAA partially dehydrates to form mesityl oxide (MO) and water. The study showed that the RDR process is the superior process in terms of DAA-MO selectivity, catalyst productivity and separation costs. The main disadvantage of the CD process is the severe catalyst-liquid mass transfer resistance of the CD column and the inability to control temperature independently from pressure.

L12 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Iron-containing silicalites for phenol catalytic wet peroxidation

AU Crowther, Nicolas; Larachi, Faical

SO Applied Catalysis, B: Environmental (2003), 46(2), 293305

CODEN: ACBEE3; ISSN: 0926-3373

AB Heterogeneous catalytic wet peroxidn. (CWPO), involving the mineralization

(i.e. complete conversion to CO₂ and H₂O) of organic compds. is a possible path for the treatment of toxic and/or bio-refractory wastewater streams. The aim of the present work was to synthesize and characterize five solid-phase catalyst formulations featuring iron(III) species supported on silica-based mesoporous mol. sieves of the MCM-41 and HMS-types. These materials were tested for the CWPO of aqueous phenol in

a

batch slurry reactor using hydrogen peroxide, as an oxidant, under very mild conditions (P=1 atm and T=80°). The five materials were produced according to four recipes. Structural data was provided by XRD and nitrogen adsorption-desorption, the iron content was assessed by atomic absorption. The freshly obtained catalysts, with embedded templates within pores, were activated either by calcination or through solvent extraction, then used for CWPO. The spent catalysts were recovered and characterized before thermal re-activation and re-exposure to fresh phenol-containing solns. For all materials, in the first run, the conversion of phenol was total and rapid (less than 15 min), and the removal of total pollution plateaued between 55 and 85% in 180 min with mineralization selectivities of ca. 95%. The materials underwent leaching of the iron, from 6% (weight/weight) to total. It was possible to perform successful CWPO reactions with some recycled materials. In terms of activity as well as robustness in the reaction conditions, one catalyst was able to remove 81% of the organic load with a selectivity of 93%, and simultaneously leaching 6% iron off. During the second run, it showed less activity but endured 2% leaching only. Surprisingly, the structure of this best catalyst was not mesoporous nor microporous and exhibited a very low sp. surface area.

L12 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI A highly active and reusable heterogeneous catalyst for the Suzuki reaction: synthesis of biaryls and polyaryls

AU Paul, Satya; Clark, James H.

SO Green Chemistry (2003), 5(5), 635-638

CODEN: GRCHFJ; ISSN: 1463-9262

AB A novel silica supported palladium catalyst has been prepared and investigated for the Suzuki cross-coupling reaction between aryl bromides and benzenboronic acid in the presence of K₂CO₃ as base and o-xylene as solvent. The key features of the catalyst include rapid reactions with 100% conversion of aryl bromides, excellent catalyst recyclability and total stability under the reaction conditions (passes hot filtration test successfully). No change in the catalyst structure has been observed on the basis of surface anal. and simultaneous thermal anal. even after the 7th use. The catalyst can be used for consecutive Suzuki reactions in a single step and hence successfully applied to the synthesis of polyaryls.

L12 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Operando resonance Raman spectroscopic characterization of the oxidation state of palladium in Pd/<SYM103>-Al₂O₃ catalysts during the combustion of methane

AU Demoulin, Olivier; Navez, Michael; Gaigneaux, Eric M.; Ruiz, Patricio;

Mamede, Anne-Sophie; Granger, Pascal; Payen, Edmond

SO Physical Chemistry Chemical Physics (2003), 5(20), 43944401

CODEN: PPCPFQ; ISSN: 1463-9076

AB Resonance Raman spectroscopy is used in order to investigate the behavior of Pd/<SYM103>-alumina (2 weight%) in the catalytic combustion of methane.

Simultaneous spectroscopic and catalytic measurements allow an operando spectroscopic investigation of the catalyst

under operational conditions. Temperature cycles were performed by alternately

heating and cooling the system under the reaction conditions after various in situ gaseous pretreatments of the catalyst. Neither the Raman features nor the conversion of methane are influenced by initial thermal activation treatment under reducing or oxidizing atmospheres. Pure metallic palladium was inactive for the catalytic combustion of methane. Under the reaction conditions, the Pd/<SYM103>-Al₂O₃ catalyst is always in an oxide PdO form with its surface in an intermediate state between surface lacunary PdO and crystalline PdO species.

L12 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Catalytic Raman spectroscopy: the operando approach

AU Banares, Miguel A.

SO Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), COLL-078 Publisher: American Chemical

Society, Washington, D. C.

CODEN: 69EKY9

AB Raman spectroscopy can provide fundamental information about the catalytic

mol. structures and surface reaction intermediates under in situ conditions. The combination of fundamental mol. structural information and in situ capabilities has resulted in an explosion of Raman spectroscopy studies in catalysis that began in the 1970s. There has been an increasing emphasis on the mol. characterization of catalysts under reaction conditions since such fundamental information should lead to the development of mol. structure-activity/selectivity relationship. Presently, this is resulting in Raman studies of catalysts under real reaction conditions, where structure and activity/selectivity are measured simultaneously; for the sake of simplicity, this in situ spectroscopy under genuine reaction conditions is given the name "operando". A critical view of the evolution in Raman spectroscopy from in situ to operando is presented.

L12 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Selective Oxidation of Propylene to Propylene Oxide by Molecular Oxygen over Ti-Al-HMS Catalysts

AU Liu, Yanyong; Murata, Kazuhisa; Inaba, Megumu; Mimura, Naoki

SO Catalysis Letters (2003), 89(1-2), 49-53

CODEN: CALEER; ISSN: 1011-372X

AB Ti- and Al-containing hexagonal mesoporous silicas (HMS) were synthesized at

ambient temperature using dodecylamine as surfactant, and the resultant compds.

were used as catalysts for the oxidation of propylene by mol. oxygen.

Ti-Al-HMS, which was prepared by reaction of Ti(iso-OC₃H₇)₄, Al(iso-OC₃H₇)₃

and SiOC₂H₅)₄ in an alc.-aqueous solution in the presence of dodecylamine, showed

47.8 of conversion and 30.6 of selectivity for propylene oxide (PO) at 523 K. The yield of PO over Ti-Al-HMS (14.6) was much higher than those over Ti-HMS (1.3) and Al-HMS (0.9) at the same reaction conditions. Ti-Al-HMS was also e more effective for PO formation than the supported catalysts (Ti/Al-HMS and Al/Ti-HMS) prepared by impregnation method. These results indicated that the simultaneous existence of Ti and Al in HMS was very important for improving the yield of PO from the oxidation of propylene, and the synthesis method influenced the catalytic activity of the Ti- and Al-containing HMS catalysts.

L12 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Production of diethyl carbonate from ethanol and carbon monoxide over a heterogeneous catalytic flow reactor

AU Roh, Nam-Sun; Dunn, Brian C.; Eyring, Edward M.; Pugmire, Ronald J.; Meuzelaar, Henk L. C.

SO Fuel Processing Technology (2003), 83(1-3), 27-38

CODEN: FPTEDY; ISSN: 0378-3820

AB Di-Et carbonate (DEC) is a candidate for use as an oxygen-containing additive

in gasoline and diesel fuel to diminish pollutant emissions. The synthesis of DEC by the oxidative carbonylation of ethanol in the gas phase over heterogeneous CuCl₂/PdCl₂ catalysts supported on activated carbon (AC) has been investigated by using a laboratory-scale continuous flow

reactor with online GC/MS. Influences of various reaction

conditions and catalyst pretreatment on the DEC yield and selectivity have been tested. Yield of DEC at 150 °C reached a maximum of 12.5 weight% and was found to increase with an increase of residence time, reaction temperature, and reaction pressure as expected. The relationship between CO flow rate and production of DEC showed

three distinct regions of DEC production. A byproduct, diethoxymethane, was formed when ethanol was introduced in stoichiometric excess.

Catalyst pretreated with KOH presented the best catalytic performance, and all metal hydroxides tested enhanced the yield of and selectivity for DEC simultaneously. However, the CuCl₂/PdCl₂/AC-KOH catalyst with a higher OH/Cu mole ratio than 2.0 showed an even lower DEC yield than that found by using a CuCl₂/PdCl₂/AC catalyst without KOH.

L12 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Synthesis of 2-methyl-3-(3,4-methylenedioxyphenyl)acraldehyde by KF/Al₂O₃ catalyst

AU Ma, Xin-bin; Huang, Zong-liang; Na, Pin; Li, Liang-long; Yu, Yan-dong
SO Sichuan Daxue Xuebao, Gongcheng Kexueban (2002), 34(5), 5658
CODEN: SXGKFI; ISSN: 1009-3087

AB 2-Me-3-(3,4-methylenedioxyphenyl)acraldehyde was synthesized through Claisen-Schmidt condensation reaction of the heliotropin and propanal over a KF/Al₂O₃ catalyst. The results indicate that the KF/Al₂O₃ catalyst is one of the best catalysts for the Claisen-Schmidt condensation. Adaptive technol. conditions have been determined by experiment. The yield of parallel experiment was 80.2% under the reaction conditions which are 60 °C, 0.3 mol heliotropin and 0.42 mol propanal as reactants, 14 g KF/Al₂O₃ catalyst, the feeding time of propanal 2 h, reaction time 2 h.

L12 ANSWER 11 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Enantioselective Total Synthesis of (-)-Strychnine Using the Catalytic Asymmetric Michael Reaction and Tandem Cyclization

AU Ohshima, Takashi; Xu, Youjun; Takita, Ryo; Shimizu, Satoshi; Zhong, Dafang; Shibasaki, Masakatsu

SO Journal of the American Chemical Society (2002), 124(49), 14546-14547
CODEN: JACSAT; ISSN: 0002-7863

GI

AB The enantioselective total synthesis of (-)-strychnine was accomplished through the use of the highly practical catalytic asym. Michael reaction of 2-cyclohexen-1-one with di-Me malonate (0.1 mol % of (R)-ALB, more than kilogram scale, without chromatog., 91% yield and >99% ee) as well as a tandem cyclization of (nitrophenyl)propenylcyclohexenone I that simultaneously constructed B- and D-rings (>77% yield). Moreover, newly developed reaction conditions for thionium ion cyclization, NaBH₃CN reduction of the imine moiety in the presence of Lewis acid to prevent ring opening reaction, and chemoselective reduction of the thioether (desulfurization) in the presence of exocyclic olefin were pivotal to complete the synthesis. The described chemical paves the way for the synthesis of more advanced Strychnos alkaloids.

L12 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI A Raman Spectroscopy Study of Alumina-Supported Vanadium Oxide Catalyst

during Propane Oxidative Dehydrogenation with Online Activity Measurement

AU Cortez, Gilberto Garcia; Banares, Miguel A.

SO Journal of Catalysis (2002), 209(1), 197-201
CODEN: JCTLA5; ISSN: 0021-9517

AB The use of an advanced in situ methodol. that combines in situ Raman spectra during catalytic operation and simultaneous online activity measurement is used to study the performance and structure of supported V oxide catalysts during propane oxidative dehydrogenation (ODH). In situ spectroscopy during reaction conditions, with online activity measurement, comprises the simultaneous use of both catalytic and spectroscopic measurement on the same sample. Thus, the possibility of assessing a structure-activity relation at a mol. level becomes reliable since the

structures observed correspond to the working catalyst, as determined online.

The

structure of supported V oxide catalyst under propane ODH is close to that of the system under dehydrated conditions but may show a very moderate extent of reduction. The extent of reduction is strongly dependent on the O₂/C₃H₈

ratio in the reaction feed. Raman spectroscopy during reaction conditions with online activity measurement shows that surface polymeric V oxide species are more reducible than isolated surface polymeric species. The reduction of surface polymeric species decreases moderately the conversion values but has no appreciable effect on the conversion and selectivity values during propane ODH reaction. Therefore, the active site for propane ODH reaction on alumina-supported vanadia must be a single VO₄ site, and no special arrangement of V sites appears to be critical. It is also discussed that the V-O-V bond may not be critical for this reaction.

L12 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Simultaneous determination of reaction kinetics and oxygen activity in single-phase oxidic catalysts and their mixture during partial oxidations

AU Estenfelder, M.; Lintz, H.-G.

SO Journal of Catalysis (2002), 209(1), 177-185

CODEN: JCTLA5; ISSN: 0021-9517

AB The partial oxidation of acrolein to acrylic acid has been studied over two single-phase oxidation catalysts and a mixture of both catalysts. One phase was mainly based on Mo and V (MoVOx); the other was a copper molybdate, CuMoO₄. The exptl. setup enabled the simultaneous determination of reaction kinetics and the oxygen activity of the catalyst under working conditions. The kinetic measurements were performed by monitoring the gas-phase composition along the length of a fixed bed of catalyst which

was

loaded into a sample port reactor. The reactor was treated as an isothermal plug-flow system. Over MoVOx the aldehyde could be oxidized to the corresponding acid with high activity and selectivity (maximum acid yield: 92 mol%). In contrast, the copper molybdate proved to be nearly inactive and unselective with respect to the acid under the same reaction conditions, with the maximum yield of the acid always being below 2 mol%. Surprisingly, the selectivity towards the acid and as a consequence the acid yield could be significantly improved (maximum acid yield: 95 mol%) by mech. mixing both catalysts. This demonstrates a synergism between the MoVOx and the copper molybdate in the case of the partial oxidation investigated. The simultaneous determination of the oxygen activity in the catalyst has been realized by use of a solid electrolyte potentiometry (SEP) cell, connected to the apparatus. The results of potentiometric measurements show that both single-phase catalysts, the MoVOx and the copper molybdate, are always in a reduced state under working conditions. As long as a significant amount of the aldehyde (>0.2 mol%) was present in the gas phase, MoVOx remained in a highly reduced state, reflecting the strong interaction between the aldehyde and the catalyst. The less reduced state of MoVOx in contact with a mixture

containing

the carboxylic acid instead of the aldehyde reflects the weaker interaction of MoVOx with the intermediate carboxylic acid. In contrast, the reduction of the copper molybdate catalyst was more pronounced in

contact

with a mixture containing the acid instead of the aldehyde. This indicates that the rate of the total oxidation of the acid is higher than the rate of its formation, which is the main reason for the low acid yields over the copper molybdate. The oxygen activity in MoVCuOx, which can be regarded as a mixture of MoVOx and CuMoO₄, lay between the values for the single oxides, which can be interpreted by the transport of oxygen from the donor-phase CuMoO₄ to the acceptor-phase MoVOx. The transferred oxygen may act as a selective species, thus increasing the selectivity of the aldehyde oxidation with respect to the corresponding acid.

L12 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Molecular structures of supported metal oxide catalysts under different environments

AU Banares, M. A.; Wachs, I. E.

SO Journal of Raman Spectroscopy (2002), 33(5), 359-380

CODEN: JRSPAF; ISSN: 0377-0486

AB A review; the use of in situ Raman spectroscopy to study the mol. structures of supported metal oxide catalysts under different environments is reviewed. The mol. structures under ambient (hydrated) and dehydrated conditions are presented. The effect of moisture at elevated temps. is also presented and discussed with regard to its implications for catalytic

phenomena. The mol. structural transformations during C2C4 lower alkane (LPG) oxidation, methane oxidation, methanol oxidation and selective catalytic reduction of NO with NH3 reaction conditions are presented. In situ spectroscopy during catalytic reaction with simultaneous activity/selectivity measurement ("operando" spectroscopy) is emphasized owing to its contribution to the fundamental understanding of catalytic performance. The reducibility of the different surface metal oxide species, the relevance of surface coverage (surface monomeric vs polymeric species) and the specific oxide support are discussed when LPG, methane, methanol or hydrogen is the reducing agent. In situ Raman spectroscopy provides mol.-level information about the surface metal oxide species: structures, stability and transformations under different environments. In many cases, the use of complementary spectroscopic techniques results in a more complete understanding of the mol. structure-activity/selectivity relationships for supported metal oxide catalysts.

L12 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Evaluation of catalytic cracking catalyst for reducing sulfur content in gasoline

AU Zheng, Junsheng; Li, Chunyi; Yuan, Qimin; Li, Min; Yang, Chaohe; Shan, Honghong; Zhang, Jianfang

SO Shiyu Daxue Xuebao, Ziran Kexueban (2002), 26(1), 88-90
CODEN: SDXZE7; ISSN: 1000-5870

AB A scheme for reducing the sulfur content of gasoline in catalytic cracking process was proposed, and the catalytic cracking catalyst DS-Z3 for removing sulfur from FCC gasoline was developed. The desulfurization effect of catalyst was evaluated on a fluidized-bed apparatus. Under appropriate ratio of DS-Z3 to FCC catalyst and reaction conditions, over 30% sulfur could be reduced in comparison with only FCC catalyst being applied, and the yield of gasoline as well as the yield of C3+C4 could be improved simultaneously. The DS-Z3 catalyst had excellent properties of desulfurization and hydrocarbon cracking activity. The alkene content in gasoline could be reduced, and its octane number could be raised by adding DS-Z3 catalyst in catalytic cracking process.

L12 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Catalytic Reduction of NO and N2O to N2 in the Presence of O2, C3H6, SO2, and H2O

AU Christoforou, S. C.; Efthimiadis, E. A.; Vasalos, I. A.

SO Industrial & Engineering Chemistry Research (2002), 41(9), 2090-2095
CODEN: IECRED; ISSN: 0888-5885

AB The reduction of NO and N2O to N2 under the same reaction conditions was studied. When both NO and N2O coexisted in the feed, the two gases were reduced at different temps. over Rh- or Ru/Al2O3. NO was reduced over In/Al2O3 and N2O over Ru- or Rh/Al2O3 in the same temperature range. Bimetallic catalysts consisting of both In and Ru sites were not efficient for simultaneous NO and N2O reduction because C3H6 was oxidized over the Ru sites. A two-layered catalytic bed made of In/Al2O3 located close to the feed inlet and Ru/Al2O3 located close to the reactor exit was used to efficiently reduce (more than 80% conversion) both NO and N2O at 450°. The performance of the same catalytic system was tested by adding both H2O and SO2 in the feed. These gases caused a moderate inhibition in the activity, thus shifting the conversion vs. temperature curves to higher temps. and lowering the conversion to N2.

L12 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Microfabricated cross-flow chemical reactor for catalyst testing

AU Ajmera, Sameer K.; Delattre, Cyril; Schmidt, Martin A.; Jensen, Klavs F.

SO Sensors and Actuators, B: Chemical (2002), B82(2/3), 297-306
CODEN: SABCEB; ISSN: 0925-4005

AB A novel silicon microfabricated chemical reactor was developed for testing catalyst particles relevant to chemical process applications. The reactor incorporates a cross-flow design with a short pass multiple flow-channel geometry enabled by microfabrication technol. The cross-flow geometry minimizes pressure drop through the particle bed and yields reaction conditions desirable for the extraction of chemical kinetics. Flow distribution is achieved through an array of 256 shallow pressure drop channels that minimize the effect of the catalyst packing on the flow in the reactor. Combined expts. and modeling confirm the even distribution of flow across the wide catalyst bed with a pressure drop .apprx. 1600 times smaller than typical microfabricated packed-bed configurations. Coupled with the inherent heat and mass transfer

advantages at the sub-millimeter length scales achievable through microfabrication, the cross-flow microreactor, with an isobaric catalyst bed free of transport limitations, is an advantageous design for catalyst testing. Kinetic studies with carbon monoxide oxidation as a model reaction demonstrate the usefulness of the microreactor for testing catalysts. When instrumented with sensors, the silicon cross-flow microreactor provides the opportunity for parallel, high-throughput testing of heterogeneous catalysts.

L12 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI The methane reforming with carbon dioxide on Ni-catalyst activated by a DC-pulsed corona discharge

AU Hong, Suk-Won; Oh, Seung-Min; Park, Dong-Wha; Kim, Geon-Joong

SO Journal of Industrial and Engineering Chemistry (Seoul, Republic of Korea) (2001), 7(6), 410-416

CODEN: JIECFI; ISSN: 1226-086X

AB CO2 reforming of CH4 to the synthesis gas was investigated in a DC pulsed corona discharge with or without the presence of Ni catalyst. It was established that the corona discharge could effectively lower the reaction temperature range of optimum catalytic performance for reforming. The synergy

effect could be found in the simultaneous presence of corona discharge and Ni-catalyst for the conversion of methane and carbon dioxide. The synthesis gas yield was enhanced with increasing DC source voltage and resistance time. The higher conversion values were obtained by using Ni-supported on NaX zeolite itself as a catalyst or in conjunction with corona discharge. The obtained synthesis gas was used as a reactant to produce DME under the elevated pressure up to 20 atm, and the effects of reaction conditions and the type of hybrid catalyst were also examined. For the synthesis of DME, Cu/Zn/HY exhibited an efficient catalytic property as compared with more acidic H-Mordenite catalyst.

L12 ANSWER 19 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Automated Library Generation Using Sequential Microwave-Assisted

Chemistry. Application toward the Biginelli Multicomponent Condensation

AU Stadler, Alexander; Kappe, C. Oliver

SO Journal of Combinatorial Chemistry (2001), 3(6), 624-630

CODEN: JCCHFF; ISSN: 1520-4766

AB The concept of automated sequential microwave-assisted library synthesis is introduced. For this purpose a dedicated single-mode microwave reactor with a robotics interface including a liquid handler and gripper was employed. The liquid handler allows dispensing of reagents into the Teflon sealed reaction vials, while the gripper moves each sealed vial in and out of the microwave cavity after irradiation. This technol. was employed for the Biginelli three-component cyclocondensation reaction. A diverse set of 17 CH-acidic-carbonyl compds., 25 aldehydes, and 8 urea/thioureas was used in the preparation of a dihydropyrimidine (DHPM) library. Out of the full set of 3400 possible DHPM derivs., a representative subset of 48 analogs was prepared using automated addition of building blocks and subsequent sequential

microwave irradiation of each process vial. For most building block combinations 10 min of microwave flash heating at 120 °C using AcOH/EtOH (3:1) and 10 mol % Yb(OTf)3 as solvent/catalyst system proved to

be successful, leading to an average isolated yield of 52% of DHPMs with >90% purity. Lanthanum (III) chloride was the preferred catalyst for Biginelli condensation reactions of thioureas. Sequential microwave-assisted processes, unlike parallel processes, allow the modification of reaction conditions for some building block combinations, for example, changes in the solvent, catalyst, reaction temperature, or irradiation time. When the unattended automation capabilities of the microwave synthesizer are used, a 48-membered library can be synthesized within 12 h.

L12 ANSWER 20 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Structural change and catalytic activity of horseradish peroxidase in oxidative polymerization of phenol

AU Akita, Masaru; Tsutsumi, Daisuke; Kobayashi, Masami; Kise, Hideo

SO Bioscience, Biotechnology, and Biochemistry (2001), 65(7), 1581-1588
CODEN: BBBIEJ; ISSN: 0916-8451

AB The effects of solvent and reaction conditions on the catalytic activity of horseradish peroxidase (HRP) were investigated for oxidative polymerization of phenol in water/organic mixts. using hydrogen peroxide

as an oxidant. Also, the structural changes of HRP were investigated by CD and absorption spectroscopy in these solvents. The results suggest that the yield of phenol polymer (the conversion of

phenol to polymer) is strongly affected by the reaction conditions due to the structural changes of HRP, i.e., the changes in higher structure of the apo-protein and dissociation or decomposition of the prosthetic heme. Optimum solvent compns. for phenol polymerization depend on the nature of the organic solvents owing to different effects of the solvents on HRP structure. In addition to initial rapid changes, slower changes of HRP structure occur in water/organic solvents especially at high concns. of organic solvents. In parallel with these structural changes, catalytic activity of HRP decreases with time in these solvents. At higher reaction temps., the yield of the polymer decreases, which is also ascribed to modification of HRP structure. It is known that hydrogen peroxide is an inhibitor of HRP, and the yield of phenol polymer is strongly dependent on the manner of addition of hydrogen peroxide to the reaction solns. The polymer yield decreases significantly when hydrogen peroxide was added to the reaction solution in a large amount at once. This is probably due to inactivation of HRP by excess hydrogen peroxide. From the CD and absorption spectra, it is suggested that excess hydrogen peroxide causes not only decomposition of the prosthetic heme but also modification of the higher structure of HRP.

L12 ANSWER 21 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Study on hydroetherification of FCC light gasoline using Pd/ion exchanger resin catalyst

AU Wang, Haiyan; Zhou, Ding

SO Lizi Jiaohuan Yu Xifu (2001), 17(3), 217-223

CODEN: LJYXE5; ISSN: 1001-5493

AB The hydroetherification of FCC light gasoline was studied using Pd/D005 cationic exchange resin catalyst. The selective hydrogenation of diolefin and the etherification of tertiary carbonic olefins with methanol can be catalyzed simultaneously. The yield of ether was up to 55.32% under the conditions: reaction temperature 343 K, pressure 1.5 MPa, molar ratio of methanol to tertiary carbonic olefins 1.1, that of hydrogen to diolefin 2, and space velocity 3/h. The lifetime test for 2016h showed that the activity of the catalyst was very stable, which can be used over a long period of time.

L12 ANSWER 22 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI In situ studies of atomic, nano- and macroscale order during VOHPO4-0.5H2O transformation to (VO)2P2O7

AU Gulians, V. V.; Holmes, S. A.; Benziger, J. B.; Heaney, P.; Yates, D.; Wachs, I. E.

SO Journal of Molecular Catalysis A: Chemical (2001), 172(12), 265-276
CODEN: JMCCF2; ISSN: 1381-1169

AB Transformation of VOHPO4-0.5H2O precursor to well-crystallized (VO)2P2O7, for n-butane oxidation to maleic anhydride was studied by in situ Raman and XRD techniques. Atomic scale changes observed in the precursor structure at 583 K provided new insights into its transformation to (VO)2P2O7. In addition to (VO)2P2O7, nanocryst. oxidized <SYM100>-VOPO4

invisible to XRD was detected during transformation in n-butane/air, possibly due to the specificity of the in situ conditions. Under catalytic reaction conditions the disordered nanocryst. (VO)2P2O7 in the fresh catalysts (ca. 10-20 nm domains) gradually transformed into well-crystallized (VO)2P2O7 in the equilibrated VPO

catalysts (>30 nm domains) with time on stream. Simultaneously, a disordered layer ca. 2 nm thick which was covering the surface (1 0 0) planes of (VO)2P2O7 disappeared yielding a solid with high steady-state catalytic performance. Only (VO)2P2O7 was observed both at room temperature and reaction temperature in the equilibrated VPO catalysts.

Sp. surface termination of the (1 0 0) planes of (VO)2P2O7 in the equilibrated VPO catalysts is believed to be responsible for high activity and selectivity of these catalysts for maleic anhydride formation.

L12 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Parallel catalyst screening instrumentation

AU Andrews, Kara; Hsiao, Gregor

SO Chimica Oggi (2001), 19(3/4), 53-55

CODEN: CHOGDS; ISSN: 0392-839X

AB A well-designed parallel pressure reactor system which employs multiple small scale reactors can be employed to optimize catalytic reactions such as hydrogenation, carbonylation, and olefin polymerization. Proper implementation of parallel technol. results in a cost effective compact unit which increases the efficiency and still allows sufficient flexibility for difficult research,

yielding accurate and reliable data for the evaluation of appropriate catalytic reaction conditions.

L12 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI An experimental and theoretical investigation of a catalytic membrane reactor for the oxidative dehydrogenation of methanol

AU Brinkmann, T.; Perera, S. P.; Thomas, W. J.

SO Chemical Engineering Science (2001), 56(6), 2047-2061

CODEN: CESCAC; ISSN: 0009-2509

AB The catalytic oxidation of methanol was investigated employing a tubular wall

reactor to elucidate reaction kinetics and a membrane reactor to record performance. The membrane reactor consisted of a composite multilayered ceramic tube impregnated with platinum catalyst and housed within a shell of stainless steel construction. Thermodyn. calcns. and catalyst activity expts. revealed that hydrogen is a main product of reaction for mixts. rich in methanol and lean in oxygen for temps. up to 300° and 1 bar pressure. Kinetic expts. indicated that two sep. pathways yielding hydrogen were prevalent: a catalytic dehydrogenative oxidation giving H2 and CO2 as products and complete catalytic combustion giving CO2 and H2O. Further exptl. measurements using the catalytic membrane reactor showed that hydrogen as product could be partially

separated

from the reaction products by the action of the ceramic membrane. A comprehensive theor. model of the membrane reactor was constructed using Maxwell-Stefan equations, the dusty gas model and differential energy balances. Results of the theor. investigation utilizing the kinetic parameters found by experiment indicated reasonably good agreement between

theory and experiment. However, it was also clear that using a ceramic membrane

impregnated with catalyst is not an efficient way to achieve H2 separation during reaction on account of the ability of H2 under the prevailing reaction conditions to diffuse in opposite directions simultaneously.

L12 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Unraveling catalytic kinetics via detailed mechanistic modeling and computational chemistry.

AU Broadbelt, Linda J.; Dooling, David J.; Klinke, David J.

SO Abstracts of Papers - American Chemical Society (2000), 220th, PHYS-132

CODEN: ACSRAL; ISSN: 0065-7727

AB Complex heterogeneous catalytic systems are ripe for the application of detailed mechanistic models to probe the relationships among catalyst structure, reaction conditions and product

selectivities. However, development of these models has been hampered, in part, by the sheer complexity of the systems of interest. Describing specific interactions of mols. and reactive intermediates with the catalyst surface demands accounting for potentially thousands of different species in various arrangements on multiple types of catalytic sites. As the population of different species on the surface changes, the interaction energies and the associated rate consts. of the transformations are also altered. These two challenges suggest that in order to make progress in developing predictive models of heterogeneous

catalytic systems, we must simultaneously improve the description of the reactive species and the quant. parameters governing their interactions. To overcome the first challenge, we have developed software for computer generation of reaction mechanisms that facilitates construction of kinetic models. Reaction mechanisms of unprecedented size and detail can be built in seconds, while manual construction of these models would be prohibitive. To address the second need, we have exploited computational chemical Quantum chemical calcns. are an

increasingly

accurate and valuable complement to exptl. studies and allow characteristics of catalytic systems to be probed that are difficult to isolate and quantify exptl. Application of our modeling approach to unravel the chemical of Fischer-Tropsch synthesis and methanation will be discussed.

L12 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Manufacture of carbonylation products, aldehydes and/or alcohols, esters

from the alcohols, ester plasticizers, and thermoplastic resins

IN Seto, Yoko; Takeuchi, Hisao; Asai, Masakazu; Sato, Tadamasu

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

AB Carbonylation products having a desired isomer distribution are manufactured by

simultaneously double bond-isomerization and carbonylation of

olefins using catalysts capable of introducing carbonyl groups into terminal olefins by controlling reaction condition. Thus, 4-octene was reacted in the presence of Rh(acac)(CO)₂ and tris(2,4-di-tert-butylphenyl) phosphite in heptane under 50 kg/cm² CO/H₂ at 100° for 30 min to give nonanol containing 4-formyloctane 60.8, 3-formyloctane 26.2, 2-formyloctane 11.6%, and 1-formyloctane 1.5% at 92.8% conversion and nonanol. Nonanol isomer mixture was reacted with phthalic anhydride in the presence of Ti(OPr)₄ at 220° to give an ester mixture, which (50 parts) was mixed with 100 parts PVC and pressed to give a sheet having tensile strength 183 kg/cm² and 100% modulus 75 kg/cm².

L12 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Shape-selective synthesis of 4,4'-dimethylbiphenyl. I. Methylation of 4-methylbiphenyl over modified zeolite catalysts

AU Shen, Jian-Ping; Sun, Lu; Song, Chunshan

SO Catalysis Letters (2000), 65(1-3), 147-151

CODEN: CALEER; ISSN: 1011-372X

AB Methylation of 4-methylbiphenyl with methanol was carried out using zeolites HY, HM, and HZSM-5 as catalysts under fixed-bed down-flow conditions. HY and HM display no shape selectivity, but HZSM-5 shows moderate selectivity to the target product, 4,4'-dimethylbiphenyl (I) under proper reaction conditions. Modification of the surface of HZSM-5 zeolite can improve the selectivity for I, especially the simultaneous modification of external and internal surfaces of the zeolite catalysts with inorg. P compound, particularly ammonium hydrogen phosphate. The selectivity for I can be increased to as high as 65% by using HZSM-5 modified with a small amount of ammonium hydrogen phosphate as the methylation catalyst.

L12 ANSWER 28 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Activity, Selectivity, and Sulfur Resistance of Pt/WO_x-ZrO₂ and Pt/Beta Catalysts for the Simultaneous Hydroisomerization of n-Heptane and Hydrogenation of Benzene

AU Arribas, M. A.; Marquez, F.; Martinez, A.

SO Journal of Catalysis (2000), 190(2), 309-319

CODEN: JCTLA5; ISSN: 0021-9517

AB Bifunctional Pt/WO_x-ZrO₂ (Pt/WZr, 12.7 wt% W) and Pt/Beta (Si/Al=12) catalysts have been studied for the simultaneous n-alkane hydroisomerization and aromatic hydrogenation using a n-heptane/benzene feed mixture (25 wt% benzene) at 3.0 MPa and temps. in the

473-573 K range. The catalysts were characterized by X-ray diffraction, adsorption-desorption of N₂, laser Raman spectroscopy (for WZr), temperature-programmed desorption (TPD) of NH₃, CO chemisorption, temperature-programmed reduction (TPR), and XPS. In the absence of sulfur, the

Pt/WZr catalyst was more active than Pt/Beta, indicating that the former has some acid sites of a higher acid strength, as suggested also by NH₃-TPD. At constant n-C₇ conversion, the selectivity to iso-C₇ was similar for both catalysts (ca. 87% for Pt/Beta and 90% for Pt/WZr at 75% conversion), but the concentration of high octane di+tribranch C₇ isomers was slightly higher for Pt/WZr. Under the reaction conditions used, benzene was totally hydrogenated on both catalysts, with a selectivity to cyclohexane (CH)+methylcyclopentane (MCP) above 90%. The MCP/CH ratio was

higher for Pt/Beta. In the presence of 200 ppm sulfur, the Pt/Beta catalyst retained a much higher isomerization activity than Pt/WZr. Furthermore, the conversion of benzene was kept at 100% for the zeolite-based catalyst in the range of TOS studied, while it decreased from 100% to ca. 0 and 4% after ca. 300 min on stream for Pt/WZr samples containing 0.6 and 1% Pt, resp. The lower sulfur resistance of Pt/WZr could be explained by a too strong interaction of part of the Pt with surface W⁶⁺ species in the WO_x-ZrO₂ support, as evidenced by TPR and XPS measurements, although the possibility of a different deactivation mechanism for both Pt/Beta and Pt/WZr catalysts and/or the formation of sulfur-resistant electron-deficient Pt species in the zeolite cavities cannot be discarded. Deactivation of the hydrogenation sites in the presence of sulfur was a reversible process for the two catalysts, while the loss of isomerization activity was seen to be almost reversible for Pt/Beta and irreversible for Pt/WZr. (c) 2000 Academic Press.

L12 ANSWER 29 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Hydrodechlorination and hydrodearomatization of monoaromatic chlorophenols

into cyclohexanol on Ru/C catalysts applied to water depollution.

Influence of the basic solvent and kinetics of the reactions

AU Felis, Vincent; De Bellefon, Claude; Fouilloux, Pierre; Schweich, Daniel

SO Applied Catalysis, B: Environmental (1999), 20(2), 91400

CODEN: ACBEE3; ISSN: 0926-3373

AB Catalytic hydrodechlorination and hydrodearomatization of 13 different mono-, di-, tri-, tetra- and pentachlorophenols were carried out simultaneously under mild reaction conditions (298-353 K, 0.3-0.5 MPa). Exptl. conditions suitable for complete conversion of the pollutants into nontoxic cyclohexanol and sodium chloride were first determined using a com. Ru/C catalyst. A new supported ruthenium catalyst was then designed that possesses a carbonaceous support suitable to concentrate chlorophenol through adsorption. Using

parachlorophenol

as a model mol., the influence of the base concentration in solution and the kinetics of the reaction under chemical regime were studied. A p-chlorophenol phenol cyclohexanol consecutive kinetic scheme was considered that drove to numerous possible kinetic models. A dynamic simulation software was used both for helping in model discrimination and for kinetic parameter estimation. The estimated activation energy values amount to

ca. 45.0±2.7 and 33.2±2.4 kJ mol⁻¹ for the hydrodechlorination and the hydrodearomatization steps, resp.

L12 ANSWER 30 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Experimental study on selectivities of Fischer-Tropsch synthesis over a Fe-Cu-K catalyst

AU Ma, Wemping; Zhao, Yulong; Li, Yongwang; Xu, Yuanyuan; Zhou, Jinglai

SO Tianranqi Huagong (1998), 23(3), 1-6

CODEN: THTKEF; ISSN: 1001-9219

AB The selectivities to products of Fischer-Tropsch (FT) synthesis over an industrial Fe-Cu-K catalyst are investigated in a fixed-bed reactor by changing reaction conditions. The FT and water gas shift (WGS) reactions take place simultaneously on the catalyst surface, and product distributions varied with operation conditions. With increasing temperature, from 503 to 543 K, the selectivities to and yields of methane and light hydrocarbons increased, but the yield of wax and the olefin-paraffin (O/P) ratio decreased. The influence of H₂-CO ratio in the feed gas on selectivities to FT products was also investigated. Increasing the H₂-CO ratio, from 1.02 to 2.83, can increase the selectivities to methane and C₂-4-hydrocarbons, but decreased the space-time yields of oil and wax and the O/P ratio. Pressure is one of the important factors that influence product selectivities of FT synthesis.

L12 ANSWER 31 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Effect of cobalt chloride on the regioselectivity of reaction of olefins with carbon monoxide and alcohols, catalyzed with PdCl₂(Ph₃P)₂

AU Kron, T. E.; Terekhova, M. I.; Noskov, Yu. G.; Petrov, E. S.

SO Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (1997), 67(1), 102-105

CODEN: RJGCEK; ISSN: 1070-3632

AB CoCl₂ additives increase the regioselectivity of the reaction of 1-heptene and styrene with CO and MeOH or BuOH to give linear esters catalyzed by PdCl₂(Ph₃P)₂, with a simultaneous increase in the total product yield. The effect of CoCl₂ is the most pronounced in hydrocarboalkoxylation of styrene in hexane; in the presence of the promoter the isomeric composition of the reaction product becomes inverse. The causes of such an effect of CoCl₂ are discussed in terms of the formation of Co(I) complexes under the reaction conditions.

L12 ANSWER 32 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Effect of the addition of chromium- and manganese oxides on structural and catalytic properties of copper/zirconia catalysts for the synthesis of methanol from carbon dioxide

AU Kilo, M.; Weigel, J.; Wokaun, A.; Koeppl, R. A.; Stoeckli, A.; Baiker, A.

SO Journal of Molecular Catalysis A: Chemical (1997), 126(23), 169-184

CODEN: JMCCF2; ISSN: 1381-1169

AB The effect of Cr oxides and Mn oxides on the structural and catalytic properties of copper/zirconia used for methanol synthesis from carbon dioxide and hydrogen has been investigated by several techniques (TG/DTA, XRD, TPR, XPS, N₂O titration, nitrogen physisorption). The methanol selectivity of all catalysts is governed by the competition of the simultaneously catalyzed methanol synthesis and reverse water gas shift reaction. The chromium-containing sample produces predominantly methanol, whereas the manganese-containing catalyst is most active for CO formation. For reaction temps. 443-513 K

and 1.7 MPa total pressure, methanol formation decreases in the order Cu/ZrO₂>Cu/CrO_x/ZrO₂>Cu/MnO_x/ZrO₂ for catalysts dried at 403 K. After calcination at 623 K in air, methanol synthesis activity is similar for all catalysts. For temps. >523 K, Cu/CrO_x/ZrO₂ shows the highest activity for methanol production. The addition of chromium oxide and (less pronounced) manganese oxide to Cu/ZrO₂ retards sintering of the copper component and shifts the crystallization of amorphous zirconia to higher temps., thus, resulting in an increased thermal stability of the catalyst under reaction conditions. XPS was applied to examine the relative surface concns. and the oxidation state of the catalyst components. XPS shows that there is no apparent correlation between the oxidation states of the metals and the catalytic properties of the catalysts. In situ diffuse reflectance FTIR studies were performed to identify the species present on the catalyst surface under CO₂ hydrogenation conditions and to elucidate the reaction mechanism. With all catalysts, surface carbonate and formate species were formed rapidly. Evidence is given that over copper/zirconia based catalysts methanol is formed mainly from bidentate surface carbonate via adsorbed CO, <SYM112>-bound formaldehyde, and surface-bound methylene.

L12 ANSWER 33 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Oxidative coupling of methane over SrF₂/Y₂O₃ catalyst

AU Long, R. Q.; Wan, H. L.

SO Applied Catalysis, A: General (1997), 159(12), 45-58

CODEN: ACAGE4; ISSN: 0926-860X

AB The use of SrF₂ as a dopant of Y₂O₃ catalyst for oxidative coupling of methane apparently increased C₂ selectivity and yield under the same conditions. However, it simultaneously decreased both the acidity and basicity of the catalyst, indicating that there was no direct relationship between catalytic performance and acidity/basicity of the catalyst. The interaction between SrF₂ and Y₂O₃ phase took place more or less in the course of the catalyst prepns., as proved by XRD results of the fresh and used catalysts. The intrinsic anionic vacancies in the catalyst would be favorable to the activation of mol. oxygen under the reaction conditions.

ESR and in situ Raman spectral results showed that superoxide ion (O⁻²) species was observed on the surface of O₂-pretreated 67 mol% SrF₂/Y₂O₃ catalyst at 973 K, which may be the active oxygen species for oxidative coupling of methane.

L12 ANSWER 34 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Analytical derivatizations of volatile and hydrophilic carbonyls from aqueous matrix onto a solid phase of a polystyrene-divinylbenzene macroreticular resin

AU Breckenridge, Susan M.; Yin, Xia; Rosenfeld, Jack M.; Yu, Y. H.

SO Journal of Chromatography, B: Biomedical Sciences and Applications (1997),

694(2), 289-296

CODEN: JCBEP; ISSN: 0378-4347

AB Extraction and derivatization of carbonyls to benzyloximes, pentafluorobenzyloximes or 2,4-dinitrophenylhydrazones is simplified and reaction times are substantially reduced by simultaneous sorption and derivatization from aqueous solution onto a solid phase. In this reaction a macroreticular polystyrene-divinylbenzene resin acts as a sorbent and catalyst to allow simultaneous extraction and derivatization of hydrophilic and lipophilic aldehydes and ketones from simple as well as complex matrixes including plasma. Conversion to the 2,4-dinitrophenylhydrazones or pentafluorobenzyloximation at ambient temperature requires 10 and 20 min, resp. These reaction conditions correspond to at least a 6-fold reduction in reaction times for derivatization of the reactive aldehydes and a 36-72-fold reduction for preparation of derivs. for the slower reacting ketones.

L12 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Partial oxidation of methane to synthesis gas using LnCoO₃ perovskites as catalyst precursors

AU Lago, R.; Bini, G.; Pena, M. A.; Fierro, J. L. G.

SO Journal of Catalysis (1997), 167(1), 198-209

CODEN: JCTLA5; ISSN: 0021-9517

AB In this work a series of cobalt-containing perovskites LnCoO₃ (Ln = La, Pr, Nd, Sm, and Gd) has been studied as catalyst precursors for the partial oxidation of methane to synthesis gas. All the perovskite precursors were prerduced in situ, producing cobalt metal finely dispersed over the rare earth sesquioxide support described here as Ln-Co-O. Of the catalyst

tested the system Gd-Co-O showed exceptionally better performance for CO and H₂ production (with methane conversion of 73% and selectivities of 79 and 81% for CO and H₂, resp., at 1009 K). The production of synthesis gas over the other catalysts decreased in the following order: Sm-Co-O » Nd-Co-O > Pr-Co-O. The catalyst La-Co-O was active for methane combustion and only traces of CO and H₂ were

observed

under the reaction conditions. XRD and XPS analyses of the catalyst La-Co-O showed that under the reaction conditions the cobalt metal is completely reoxidized, regenerating the original LnCoO₃ perovskite structure. For the reaction over Nd-CoO the cobalt is only partially reoxidized to NdCoO₃. For Gd-Co-O and Sm-Co-O, the most stable and active catalysts for the partial oxidation of methane no reoxidn. to LnCoO₃ was observed. TPR and XRD studies showed that

the perovskite NdCoO₃ is reduced in two steps, first to NdCoO_{2.5} and further to Co⁰/Nd₂O₃ and in both stages it was demonstrated that the reoxidn. with O₂ is capable of recovering the perovskite structure. TPO expts. with reduced La-Co-O, Nd-Co-O, Sm-Co-O, and Gd-Co-O catalysts indicated that reoxidn. of cobalt also takes place in two steps: first by oxidation of the supported Co⁰ to the spinel Co₃O₄ (Co₂+Co₃+2O₄) followed by a further oxidation of the Co²⁺ to Co³⁺ with a simultaneous solid state reaction with Ln₂O₃, regenerating the perovskite structure. It was observed that the temperature for the second oxidation

step is strongly dependent on the nature of the lanthanide. Based on these results it is proposed that the deactivation of the catalysts Ln-Co-O by reoxidn. of cobalt metal is related to the thermodyn. stability of the parent perovskite structure. We also present evidence that hydroxyl groups on the rare earth oxide, specially in the La-Co-O system, might make some contribution to the reoxidn. of cobalt metal during the reaction via a reverse spillover process.

L12 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Reaction engineering studies in a polytropic fixed-bed reactor over a highly active and selective catalyst for oxidative methane coupling

AU Mleczko, Leslaw; Gayko, Guido; Niemi, Vesa M.; Hiltunen, Jyrki

SO Chemical Engineering & Technology (1997), 20(1), 29-35

CODEN: CETEER; ISSN: 0930-7516

AB The oxidative coupling of CH₄ (OCM) was carried out in a polytropic fixed-bed reactor applying a Zr/La/Sr catalyst. Over this catalyst the OCM reaction follows a complex reaction scheme which includes primary parallel reaction steps to CO, CO₂, C₂H₆, and consecutive reactions of ethane to ethylene or CO_x. Yield of higher hydrocarbons C₂+, strongly depended on reaction conditions, i.e. low partial pressures of CH₄ and O₂ obtained by diluting the feed gas with N₂ and high reaction temps. promoted C₂+ selectivity and yield. The maximum yield amounted to 21.4% (20 volume% CH₄, 9 volume% O₂, 71 vVol.-% N₂, T = 860°; XCH₄ = 41.8%, SC₂+ = 52.5%). This result belongs to the highest yields reported in the open literature.

L12 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Catalytic behavior of multiphasic oxide catalysts containing lanthanides (La, Ce, Pr, Sm, Tb) in the selective oxidation of isobutene to methacrolein

AU De Smet, F.; Ruiz, P.; Delmon, B.; Devillers, M.

SO Catalysis Letters (1996), 41(3,4), 203-207

CODEN: CALEER; ISSN: 1011-372X

AB The catalytic performances of five lanthanide oxides (La₂O₃, Sm₂O₃, CeO₂,

Pr₆O₁₁ and Tb₄O₇) for the selective oxidation of isobutene to methacrolein are evaluated within the framework of the remote control mechanism. Mech. mixts. of these oxides with typical donor (Sb₂O₄) or acceptor (MoO₃) phases of spill-over oxygen were prepared and tested for their activity in the isobutene-to-methacrolein oxidation at 400°C. Amongst the five lanthanide oxides tested, only CeO₂ and Pr₆O₁₁ were found to display significant cooperation effects for the investigated reaction, with enhanced yields and selectivity for partial oxidation and concomitant decrease of CO₂ production. The fresh and used catalysts were characterized by x-ray diffractometry, and the occurrence of solid state reactions between the partner oxides outside the reaction conditions was investigated in parallel in the temperature range 400-500°C. No new phase was observed in the case of the mixts. with La₂O₃, Sm₂O₃, CeO₂ and Tb₄O₇. Account taken of the absence of any new phase in the CeO₂-MoO₃ system, it can be concluded that CeO₂ is a potential donor of spill-over oxygen. The situation in the MoO₃-Pr₆O₁₁ mixts. is more complex, owing to the generation of various praseodymium

molybdates, together with the oxocarbonate Pr_2CO_5 . The latter phase was shown to have no intrinsic tendency to produce methacrolein, but it seems that some of the praseodymium molybdates present in the working catalysts may exhibit noticeable catalytic properties.

L12 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Promoter effect of cesium on C-C bond formation during alcohol synthesis from CO/H_2 over $\text{Cu}/\text{ZnO}/\text{Cr}_2\text{O}_3$ catalysts

AU Campos-Martin, J. M.; Fierro, J. L. G.; Guerrero-Ruiz, A.; Herman, R. G.; Klier, K.

SO Journal of Catalysis (1996), 163(2), 418-428

CODEN: JCTLA5; ISSN: 0021-9517

AB The effect of calcination temperature and Cs-promotion on Cu-ZnCr oxide catalyst was investigated in connection with both structural and catalytic properties in high-pressure CO hydrogenation. As revealed by TPR and XPS, the reduction of Cu is inhibited by Cs incorporation. Under typical reaction conditions, detectable Cu phases are reduced to metallic Cu. The crystal size of Cu particles increases with increasing reduction temperature, and simultaneously, Cs is segregated to the catalyst surface. MeOH and higher alc. yield was increased with Cs-doping of the catalysts.

L12 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Unique fractionation of biomass to polyols provides inexpensive feedstock for liquid fuels process

AU Robinson, J. M.; Mandal, H. D.; Burgess, C. E.; Brasher, C.; O'Hara, K.; Holland, P.

SO Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29

(1996), FUEL-090 Publisher: American Chemical Society, Washington, D. C. CODEN: 63BFAF

AB Previous work in this laboratory established a unique process that converts C5

and C6 polyols (straight chain hydrocarbons with a hydroxyl group on each carbon) to hydrocarbons using hydroiodic and phosphorous acids. In order to use renewable biomass resources as feedstock for this process, the biomass must first be fractionated (e.g. by steam explosion) for cellulose recovery; the cellulose can then be hydrolyzed and reduced to polyols. However, we have investigated a one-step Russian method to directly convert raw "biomass-to-polyols" (BTP). In this reaction, biomass is subjected to simultaneous dilute acid hydrolysis and catalytic hydrogenation, thus trapping the incipient aldoses as their corresponding, but less reactive, polyols (alditols). We have developed this method and have determined the optimum reaction conditions to obtain the highest yield of polyols, .apprx. 68% of the sawdust. Almost all of the sawdust is converted subject to mech. limitations. However, the remaining lignin byproduct is not easily separated from the catalyst. To economize this process, we are now investigating the recycle of the catalyst by removing the lignin from the spent catalyst mixture using a NaOH wash. The second and third reactions using recycled catalyst produced .apprx.58% and .apprx. 52% polyols, resp., from the sawdust. Subsequent research will assess the longevity of the catalyst and provide insight as to further procedural modifications that must be made to maintain the initial maximum conversion. Further expts. will also test this reductive-hydrolysis BTP method to convert lignite coal to liquid fuels.

L12 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Isobutane/2-butene alkylation over faujasite type zeolites in a slurry reactor. Effect of operating conditions and catalyst regeneration

AU Rorvik, Tine; Mostad, Helle; Ellestad, Ole Henrik; Stoecker, Michael

SO Applied Catalysis, A: General (1996), 137(2), 235-53

CODEN: ACAGE4; ISSN: 0926-860X

AB The isobutane/2-butene alkylation has been catalyzed by acidic cubic faujasites (H-FAU and CeY-98) and a hexagonal faujasite (H-EMT) in a semibatch slurry reactor. H-EMT exhibited the best results during the reaction with respect to an improved deactivation profile and moderate loss of alkylate selectivity compared to both CeY-98 and H-FAU. Addnl., H-EMT proved to be regenerable. The different catalytic behavior between H-EMT and H-FAU has been discussed in terms of differences in their crystal structure. Furthermore, we have focused on the influence of isobutane:2-butene molar ratio and temperature (simultaneously varied) on the catalytic behavior at constant butene WHSV fed to the slurry reactor at optimum stirring conditions. CeY-98 was used as a model catalyst and the results were treated statistically by principal component and partial least square analyses. The dependence of alkylate selectivity as well as yield related to temperature and

isobutane-2-butene molar ratio were determined. Both equations showed optima at

low butene concns., while the temperature was of minor importance. A high stirring speed was essential to achieve optimal reaction conditions enlarging the alkylate yield and selectivity.

L12 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Energy efficient methane-to-syngas conversion with low H_2/CO ratio by simultaneous catalytic reactions of methane with carbon dioxide and oxygen

AU Choudhary, V. R.; Rajput, A. M.; Prabhakar, B.

SO Catalysis Letters (1995), 32(3,4), 391-6

CODEN: CALEER; ISSN: 1011-372X

AB By simultaneous reactions of methane with CO_2 and O_2 over NiO-CaO catalyst under certain reaction conditions, it is possible to convert methane into syngas with low H_2 -CO ratio (1-2) at above 95% conversion, with 100% CO selectivity and above 90% H_2 selectivity and also with very high CO productivity without catalyst deactivation due to coking for a long period, in a most energy efficient and safe manner, requiring little or no external energy.

L12 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Gas-phase one-step preparation of 1,4-butanediol and <SYM103>-butyrolactone

IN Chu, Shiao Jung; Chen, Bo Yu; Hsu, Hsi Yen; Lin, Ching Tang; Chao, Cheng

Lun

SO Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

AB 1,4-Butanediol (I) and <SYM103>-butyrolactone (II), which are useful as raw

materials for engineering plastics, are prepared by gas-phase one-step hydrogenation-cracking which involves feeding dialkyl maleate, dialkyl succinate, or a mixture thereof to a H-containing atmospheric in the presence of Cu or

a Cu compound at 160-250°, pressure 20-70 kg/cm², feed rate 0.05-3 h-1, and the raw material/H mol ratio 20-500. Preferably the catalyst is supported on at least one carrier selected from SiO_2 , ZrO_2 , and TiO_2 and contains 20-80 weight% Cu or a Cu compound and at least one compound selected

from Ca, CaCl_2 , Zn, ZnCl_2 , K, KCl, Na, NaCl, Mn, MnCl_2 , Pd, Ba, BaO, Ni, and NiCl_2 . This process uses safe catalysts and simultaneously gives I and II in one-step. ABS modification of the Cu-based catalyst with an alkali or alkaline earth metal, Zn, Ni, Mn, or Pd or changing reaction conditions can adjust the selectivity for I (30.7-91.1%) and II (7.2-61.8%). Thus, di-Me maleate at 0.5 h-1 and H (preheated to 200°) at 9,420h-1 were introduced into a vaporization zone, mixed and vaporized, and fed into a reactor packed with a catalyst Cu-Ni/ TiO_2 - ZrO_2 at 180° and 42 atm to give I and II with 91.1 and 7.2% selectivity, resp. The catalyst Cu/ SiO_2 gave I, II, and di-Me succinate with 82.7, 10, and 1.9% selectivity, resp., under the same reaction conditions vs. 30.7, 61.7, and 2.4%, resp., when the reaction pressure was changed to 10 atmospheric

L12 ANSWER 43 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI A simplified kinetic model for Illinois No.6 coal liquefaction

AU Yamamoto, H.; Yamaura, J.; Inokuchi, K.; Ikeda, K.; Terashita, Y.; Endoh, K.

SO Conf. Proc. - Int. Conf. Coal Sci., 7th (1993), Volume 1, 287-90.

Editor(s): Michaelian, K. H. Publisher: Can. Natl. Organ. Comm., 7th Int. Conf. Coal Sci., Devon, Can.

CODEN: 61DOA4

AB A new kinetic model for the liquefaction of Illinois Number 6 coal (in 1:1 mixture of creosote oil-anthracene oil solvent and Fe sulfide catalyst) is based on the assumption that coal is decomposed to asphaltenes, followed by simultaneous decomposition of asphaltenes to oil fractions. Estimated parameters were in good agreement with exptl. results. The most effective reaction condition on product yield was the reaction temperature; the next most influential parameter was gas-slurry ratio. The reaction pressure affected the yields of hydrocarbon gas and H_2 consumption, whereas addition of catalyst affected the yields of light and middle distillate. The highest oil yield was estimated at 56 weight% (dry ash-free coal basis) using empirical formulas in this kinetic model.

L12 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

- TI Mechanism and Dynamics in the H₃[PW₁₂O₄₀]-Catalyzed Selective Epoxidation of Terminal Olefins by H₂O₂. Formation, Reactivity, and Stability of {PO₄[WO(O₂)₂]₄}³⁻
- AU Duncan, Dean C.; Chambers, R. Carlisle; Hecht, Eric; Hill, Craig L.
SO Journal of the American Chemical Society (1995), 117(2), 681-91
CODEN: JACSAT; ISSN: 0002-7863
- AB The highly selective catalytic epoxidn. of terminal alkenes by the complex WVI/PV/H₂O₂/CHCl₃/PTC (PTC = phase transfer catalyst) system (Ishii-Venturello chemical) has been extensively investigated by groups in several countries and recently commercialized, yet little is known with certainty about the mechanism. The substrate conversions and epoxide selectivities observed under biphasic conditions, aqueous H₂O₂/alkene in CHCl₃, with 21 polyoxometalates (cetylpyridinium chloride as the phase-transfer catalyst, PTC) including the Ishii precursor complex, [PW₁₂O₄₀]³⁻, clearly indicate that only [PW₁₂O₄₀]³⁻ and [PW₁₁O₃₉]⁷⁻, which both rapidly form {PO₄[WO(O₂)₂]₄}³⁻, 1, are effective.
- Simultaneous monitoring of organic oxygenated products and gaseous products (nearly all O₂) with several of these polyoxometalates confirm that H₂O₂ disproportionation is by far the dominant side reaction with several d-electron transition metal-substituted polyoxometalate catalyst precursors. Anal. of the 2JW-P coupling satellites in the 31P NMR spectra of the polytungstophosphate products from the stoichiometric reaction of 1 with alkene substrates as a function of cation, solvent, field strength, and time indicates that both a PW₄ and a PW₃ species are formed initially and one PW₂ species subsequently. Several lines of kinetic and spectroscopic evidence indicate that two processes dominate over all others during Ishii-Venturello epoxidn.: a slow epoxidn., 1 (PW₄) + alkene <SYM174> PW₄, PW₃, and PW₂ (henceforth called "subsequent peroxo species" or SPS) + epoxide, followed by a rapid regeneration of 1 with H₂O₂. First, little epoxidn. is observed until 1 is in appreciable concentration. Second, the rate law for epoxidn. of 1-octene by the Arquad salt of 1, Arq1 (Arquad = [(C₁₈H₃₇)₇S⁺ + (C₁₆H₃₃)₂]₂[CH₃]₂N⁻), in CHCl₃ at 23 °C is v₀ = k[1][1-octene]. Third, 1 is the dominant polytungstophosphate present under steady state turnover conditions. Fourth, the ratio of the initial rates of epoxidn. is v₀(ArqSPS)/v₀(Arq1) = 0.13 ± 0.01. Fifth, the dominant inorg. product in the formation of 1, { [WO(O₂)₂(H₂O)]₂O }²⁻, is two orders of magnitude slower in alkene epoxidn. than Arq1 under identical conditions at both 23 and 60 °C. Addnl. 31P NMR studies address both ion pairing effects and dynamic exchange in 1 and the SPS PW₄. A linear correlation was found between the change in both chemical shift and 2JW-P coupling constant for the SPS PW₄ species but not the SPS PW₂ or the SPS PW₃ species as a function of reaction time. This is consistent with the SPS PW₄ species undergoing rapid dynamic exchange on the 31P NMR time scale. Addition of 1 equiv of 1,2-epoxybutane to tetra-n-hexylammonium SPS (THASPS) does shift the SPS PW₄ resonance to high field with a larger 2JW-P coupling constant in accord with the correlation. Consequently, the dynamics of SPS PW₄ may reflect exchange of epoxide product. Rapid catalyst inactivation despite being one of two success limiting features of Ishii-Venturello epoxidn. was not addressed in any previous work. Under the typical biphasic reaction conditions, catalysis nearly stops after 500 turnovers. The effects of alkene, H₂O, and epoxide product on epoxidn. rates and polytungstophosphate speciation monitored by 31P NMR establish that epoxide, but apparently neither alkene nor H₂O, leads to irreversible catalyst inactivation.
- L12 ANSWER 45 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Morphology changes and deactivation of alkali-promoted Ni/SiO₂ catalysts during carbon monoxide hydrogenation
- AU Pereira, Evandro Brum; Martin, Guy-Antonin
SO Applied Catalysis, A: General (1994), 115(1), 135-46
CODEN: ACAGE4; ISSN: 0926-860X
- AB Deep morphol. transformations undergone by unpromoted and alkali-promoted Ni/SiO₂, occurring during the first hours of CO hydrogenation at atmospheric pressure, are examined using temperature-programmed hydrogenation, magnetic measurements and surface area determination. As a first step, the alkali addition results in an increase in the selectivities of CO₂, C₂+ hydrocarbons and alcs. This behavior is similar to that reported elsewhere when the reaction is performed at 5 MPa. The stability of these systems varies with the sequence K > Na > Li > unpromoted. It is shown that catalyst reduction at 873 K results in sintering of the support when alkali promoters are present, which does not alter the nickel particle size so long as the promoter concentration is not too high. The surface area of the catalysts is unchanged after reaction. The deactivation of unpromoted samples results from nickel sintering, in contrast to that of alkali-promoted catalysts: this behavior is discussed in terms of the stabilization of nickel subcarbonyl species by alkali promoters. Deactivation of promoted catalysts parallels the deposition of large amts. of carbon atoms chemical interacting with the nickel phase. In reaction conditions, alkali addition gives rise to a deep carburization of the nickel phase (up to 85%) which probably accounts for the observed change of selectivity. Two types of carbon chemical interacting with nickel are detected when alkali promoters are added. Both of them can be hydrogenated at low temperature and can be related to surface and bulk carbides.
- L12 ANSWER 46 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Hydrogenation of carbon dioxide over copper, silver and gold/zirconia catalysts: comparative study of catalyst properties and reaction pathways
- AU Baiker, A.; Kilo, M.; Maciejewski, M.; Menzi, S.; Wokaun, A.
SO Studies in Surface Science and Catalysis (1993), 75(New Frontiers in Catalysis, Pt. B), 157-72
CODEN: SSCTDM; ISSN: 0167-2991
- AB The hydrogenation of CO₂ to methanol has been investigated over group IB metal/zirconia catalysts prepared by copptn., ion exchange, and impregnation. The studies indicate that from these metals copper is most suitable for CO₂ hydrogenation to methanol. The methanol selectivity of all catalysts is governed by the competition of the simultaneously catalyzed methanol synthesis and reverse water gas shift reaction. Au/ZrO₂ is most active for the reverse water gas shift reaction and thus exhibits the lowest selectivity to methanol. Surprisingly, Cu/ZrO₂ and Ag/ZrO₂ show similar, good selectivities to methanol. Crystallization of the amorphous ZrO₂ results in significantly lower activity and selectivity with all catalysts. Thermoanal. studies of the crystallization behavior reveal that the amorphous zirconia is stabilized by the presence of copper ions, while the presence of metallic Cu, Ag or Au has no significant effect on the thermal stability of this phase. In situ diffuse reflectance FTIR studies under reaction conditions show rapid formation of surface formate on all IB metal/ZrO₂ catalysts. However, this species is not considered to be the immediate precursor to methanol. Methanol appears to be formed mainly via adsorbed CO, <SYM112>-bonded formaldehyde, and surface-bound methylate.
- L12 ANSWER 47 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Selective oxidation of methane with air over silica catalysts
- AU Sun, Qun; Herman, Richard G.; Klier, Kamil
SO Catalysis Letters (1992), 16(3), 251-61
CODEN: CALEER; ISSN: 1011-372X
- AB Partial oxidation of CH₄ by O to form HCHO, CO_x, and C₂ products (C₂H₆ and C₂H₄) was studied over SiO₂ catalyst supports (fumed Cabosil and Grace 636 silica gel) at 630-780° under ambient pressure. The catalysts exhibited high space time yields (at low conversions) for CH₄ partial oxidation to HCHO; the C₂ hydrocarbons were parallel products with HCHO. Short residence times enhanced both C₂ hydrocarbon and HCHO selectivities over formation of CO_x, even within the differential reactor regime at 780°. This suggested that the HCHO did not originate from Me radicals, but rather from MeO complexes formed from direct high-temperature chemisorption of CH₄ at the silica surface. Very high HCHO space time yields (e.g., 812 g/kg-h at space velocity 560,000 L/kg-h) could be obtained over the silica gel catalyst at 780° with a 1.5:1 CH₄-air ratio. These yields greatly surpassed those reported for silicas earlier, as well as those over many other catalysts. Low CO₂ yields were observed under these reaction conditions, with selectivities to HCHO and C₂ hydrocarbons of 28.0 and 38.8%, resp., at a CH₄ conversion of 0.7%. A reaction mechanism was proposed for the CH₄ activation over the silica surface, which can explain the product distribution patterns (especially the parallel formation of HCHO and C₂ hydrocarbons).
- L12 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
- TI Kinetics and reaction network in propane ammoxidation to acrylonitrile on vanadium-antimony-aluminum based mixed oxides
- AU Catani, Roberto; Centi, Gabriele; Trifiro, Ferruccio; Grasselli, Robert K.

SO Industrial & Engineering Chemistry Research (1992), 31(1), 107-19
CODEN: IECRED; ISSN: 0888-5885

AB The kinetics of propane (I) ammoxidn. to acrylonitrile (II) on a V-Sb-Al-based mixed oxide catalyst are described by a Langmuir-Hinshelwood approach, 6 parallel reactions of formation of II, propylene (III), C oxides, acetonitrile (IV), HCN, and C₂ hydrocarbons, 3 reactions of consecutive transformation of the intermediate III to II, IV and HCN, 5 decomposition reactions of intermediate products to C oxides, and 1 reaction of decomposition of ammonia (V). The kinetics were studied in a quartz tubular flow reactor operating both in differential and integral conditions, using I, O, and V concns. in the 0-20% range and reaction temps. of 680-810 K. II forms principally from the intermediate III, and the limiting factor in the formation of II is the relative slowness of this step compared to the others and the higher rate of III oxidation to C oxides as compared to that of II to COx. The maximum yields and selectivities to II obtained were in the 35-40 and 50-60% ranges, resp., for I conversions in the 60-80 and 40-50% ranges, resp. The relevance of the kinetic information in determining the best reaction conditions and performance using different possible feedstocks is also discussed.

L12 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Ethylene from natural gas by direct catalytic oxidation

AU Geerts, J. W. M. H.; Van Kasteren, J. M. N.; Van der Wiele, K.

SO Comm. Eur. Communities, [Rep.] EUR (1991), EUR 13061, 125 pp.
CODEN: CECED9; ISSN: 0303-755X

AB The title report describes optimizing the phys. parameters of the oxidative coupling catalyst, defining the optimum reactor design and reaction conditions, collecting data for modeling of the chemical reaction, and process design and economic evaluations. Li-doped MgO catalyst was optimized with respect to catalytic performance. Essential for the catalytic activity and selectivity is the presence of Li. The most suitable reactor was fluidized bed reactor because of the high exothermicity of the reaction. The optimum reaction conditions for reaching the maximum ethylene yield (18%) for the longest time were 800°/1 atmospheric using a CH₄/O = 5 ratio gas-feed mixture at 0.6 g-s/mL catalyst. The reaction mechanism was described as a complicated mixture of heterogeneous (catalytic) and homogeneous (gas phase) reactions occurring simultaneously. Coupling to ethane takes place in the gas phase. Ethane is dehydrogenated on the catalyst or in the gas phase to ethylene, which in turn gets easily oxidized into CO and CO₂ which are mainly formed at the catalyst surface. A computer program was developed which simulated the network reaction (>150 elementary radical reactions) of the homogeneous gas phase.

L12 ANSWER 50 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI The production of hydroxylamine by hydration of nitrate on suspended palladium/carbon catalyst: kinetics and mass transfer

AU Werner, M.; Lindner, D.; Schumpe, A.

SO Recent Trends Chem. React. Eng., [Proc. Int. Chem. React. Eng. Conf.], 2nd (1987), Volume 2, 502-17. Editor(s): Kulkarni, B. D.; Mashelkar, R. A.; Sharma, M. M. Publisher: Wiley East., New Delhi, India.
CODEN: 56IFAQ

AB The kinetics of the hydrogenation of NH₄NO₃ to NH₂OH, catalyzed by Pd on activated C, was studied in a stirred autoclave. In addition to the main reaction, the parallel hydrogenation to NH₄⁺, the consecutive hydrogenation of NH₂OH, and its catalytic decomposition are described by empirical rate equations. The selectivity of NH₂OH formation as compared to side reactions is .apprx.0.78, independent of the reaction conditions. Ammonium accelerates the hydrogenation of NH₄NO₃ and slows down the consecutive reactions by competitive adsorption on the catalyst. Gaseous byproducts (N₂O and N₂) are formed only by the decomposition of hydroxylamine in the absence of H.

L12 ANSWER 51 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Selective thermal cracking of heavy oil (Part 5). Selective thermal cracking of Kuwait atmospheric residue by using carbon monoxide shift reaction

AU Murakawa, Takashi; Fujimoto, Kaoru; Tominaga, Hiroo

SO Sekiyu Gakkaishi (1987), 30(6), 418-23
CODEN: SKGSAE; ISSN: 0582-4664

AB The cracking of Kuwait petroleum atmospheric residue was carried out in a gas-flow type autoclave reactor in the presence (or absence) of Ni/basic carrier catalysts in pressurized water gas at 420°. The thermal cracking of the residue on a Ni-Mo/Al₂O₃ catalyst is summarized

as follows: (1) the cracking and CO shift reactions proceeded simultaneously with substantial H consumption; (2) the selectivity for middle distillates increased, while that for gas and coke decreased under CO shift reaction; (3) the selectivity for middle distillates increased with increasing amount of catalyst or with increasing CO pressure; carbon monoxide (4) the level of S removal was low and the composition of the distillate was hardly affected by the catalysts and reaction conditions; (5) the hydrogenating ability of the system was lower than that of the pressurized H system.

L12 ANSWER 52 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI 1,8-Naphthalenecarbolactone and acenaphthenone in liquid-phase oxidation of acenaphthene to naphthalic anhydride

AU Tkacheva, G. D.; Suvorov, B. V.

SO Zhurnal Organicheskoi Khimii (1985), 21(6), 1289-93
CODEN: ZORKAE; ISSN: 0514-7492

AB The title compds. were major intermediates formed via parallel mechanisms in the early stages of the title oxidation with mol. O at 130° in PrCO₂H in the presence or absence of Co, Mn, and Co-Mn catalysts. The yield and ratio of the intermediates depended on the reaction conditions and the catalyst composition. The naphthalic anhydride yield increased in the order of catalysts CoBr₂ << Co(OAc)₂-KBr < PrCHO .apprx. PrCHO-Mn(OAc)₂ .apprx. Mn(OAc)₂ < Co(OAc)₂ .apprx. Mn(OAc)₂-KBr < Co(OAc)₂Mn(OAc)₂ < MnBr₂ << Co(OAc)₂-Mn(OAc)₂-KBr.

L12 ANSWER 53 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Rhodium on chromia-alumina catalysts for toluene steam-dealkylation: characteristics and catalytic behavior

AU Ferino, I.; Marongiu, B.; Torrazza, S.

SO Applied Catalysis (1984), 10(2), 125-35
CODEN: APCADI; ISSN: 0166-9834

AB Rh on Cr₂O₃/Al₂O₃ catalysts for toluene steam-dealkylation were prepared with various Cr₂O₃/Al₂O₃ ratios, Rh contents and the absence or presence of K as promoter. The catalysts were characterized by determination of total and metal surface area, pore size distribution, x-ray diffraction and ESR anal. Catalytic performances were also tested in standard conditions by a tubular flow reactor. The samples without alkali show roughly the same activity and selectivity to benzene, while coke and tar amts. decrease with increasing Cr₂O₃ weight. The activity loss data indicate a good catalyst stability, which is further improved by the addition of K. An increase in CO/CO₂ ratio is observed parallel to the progressive decrease of conversion, thus suggesting a correlation between this parameter and the catalyst stability. An interpretation of the above phenomena in terms of a proposed reaction mechanism is advanced. Under the reaction conditions <SYM103>-Al₂O₃ adsorbs H₂O predominantly by a dissociative mechanism, thus acting on the activity level of the catalyst. On the other hand, the presence on the Cr₂O₃ surface of coordinatively unsatd. Cr³⁺ ions able to adsorb mol. H₂O would enhance CO <SYM174> CO₂ transformation, thus avoiding the poisoning of the metal sites caused by strong CO adsorption.

L12 ANSWER 54 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Chloroform deuteration

IN Koch, Hans J.

SO Can., 12 pp.
CODEN: CAXXA4

AB CHCl₃ was fed continuously into a still pot, containing NaOD and catalytic tetraoctylammonium deuteroxide (I) and heated at 70-90°, whereby vapors of CHCl₃-CDCl₃ passed upward through a stainless-steel-wool-packed column countercurrent to a NaOD-D₂O-I mixture fed continuously from the column head, and the more highly deuterated CHCl₃-CDCl₃ exit vapors were divided and similarly treated in 2 parallel columns at one-half the rate of flow in the 1st column to give a product representing 99.5% conversion of CHCl₃ to CDCl₃. Spent NaOD solution was continuously withdrawn from the still pots at such a rate as to maintain the proper reaction conditions.

L12 ANSWER 55 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Hydrogenation of furfural on copper-zirconium Raney-type catalysts under hydrogen pressure

AU Erzhanova, M. S.; Beisekov, T.; Mombekov, S. A.

SO Deposited Doc. (1977), VINITI 729-77, 10 pp. Avail.: VINITI

AB Title catalysts showed high activity and selectivity for the hydrogenation of furfural to furfuryl alc.; optimal activity was observed with catalysts containing 3.0-5.0 mass% Zr. Simultaneously increasing the operating temperature and pressure increased the activity of the catalyst. The reaction order changed significantly with increasing severity of the reaction conditions.

L12 ANSWER 56 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Simultaneous manufacture of methacrylonitrile and butadiene by catalytic vapor-phase oxidation of mixed butenes

IN Yoshino, Takachika; Saito, Shigeru; Sobukawa, Masukuni; Ishikura, Jun; Sasaki, Yutaka

SO Ger. Offen., 36 pp.

CODEN: GWXXBX

AB Catalysts with the empirical formula $\text{Fe}_{10}\text{Sb}_b\text{McTe}_d\text{XeOf}$, where $\text{Mc} = \text{V}, \text{Mo},$

or $\text{W}, \text{X} = \text{P}$ and (or) $\text{B}, b = 5-60, c = 0.01-10, d = 0.03-5, e = 0-5,$ and $f = 20-225,$ were prepared and used in the vapor phase ammonoxidn. and

oxidation

of mixed butenes containing isobutene and n-butene. Thus, a catalyst with the empirical formula $\text{Fe}_{10}\text{Sb}_{25}\text{W}_{0.25}\text{Te}_{1.0}\text{O}_{67.8}(\text{SiO}_2)_3$ was prepared by adding 180

g silicic acid soluble containing 20% SiO_2 to a mixture of 11.2 g Fe powder in 81

ml HNO_3 and 100 ml H_2O and 1.3 g ammonium tungstate and 4.6 g H_6TeO_6 in 50

ml H_2O . The mixture was combined with a mixture of 60.9 g Sb in 225 ml HNO_3

and 100 ml H_2O and the pH was adjusted to 2 with NH_4OH . After evaporating the

liquid, the dry product was heated 2 hr at 200.deg. and 2 hr at 400.deg., tableted, heated 16 hr at 130.deg., and calcined for 2 hr at 900.deg..

Twenty-seven addnl. catalysts were similarly prepared. When used for the simultaneous manufacture of methacrylonitrile [126-98-7] and butadiene [106-99-0] from mixed butenes, the catalysts gave good

yields using the following reaction conditions : 350-500.deg., an O to mixed butene mole ratio of 0.5:1-6:1, an NH_3 to isobutene mole ratio of 1:1-6:1, and space velocity of the starting mixture 5000-100 hr-l.

L12 ANSWER 57 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Vapor-phase catalytic re-esterification of ethyl acetate with methanol

AU Ramachandran, Subramania; Satyanarayana, Mandavilli

SO Indian Journal of Technology (1969), 7(6), 17780

CODEN: IJOTA8; ISSN: 0019-5669

AB The continuous vapor-phase reesterification of AcOEt with methanol was studied employing a 4-stage series type integral reactor packed with a silica gel catalyst. Percentage conversions achieved under different reaction conditions (temperature 181°, 202°, 221°, and 239°; and molar ratio of MeOH to AcOEt 0.332 and 3.84) were calculated in two ways: (1) as moles of AcOMe per

100 moles reaction mixture representing the extent of the main re-esterification reaction, and (2) as moles AcOH in the product per mole AcOEt in the feed representing the extent of the combined hydrolysis and esterification side reactions. All the 3 simultaneous reactions (re-esterification, hydrolysis, and esterification) are favored on lowering the methanol content in the feed and by the presence of a catalyst with higher contact time. There is an optimum reaction temperature for the main re-esterification reaction, depending upon the feed composition; the hydrolysis reaction increases continuously with increase in temperature, irrespective of the feed composition

L12 ANSWER 58 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Relation between catalytic and electric properties of germanium and its isoelectronic analogs

AU Maidanovskaya, L. G.; Kirovskaya, I. A.

SO Tr. Tomsk. Gos. Univ., Ser. Khim. (1965), 185, 23-7

CODEN: TTUKAW

AB cf. CA 61, 8983b. The elec. conductivity, $\langle \text{SYM115} \rangle$, of Ge, GaAs, and CuBr and

their catalytic activity in the vaporphase dehydrogenation of iso-PrOH were studied simultaneously. The reaction was run in a flow system operated at .apprx.8 torr and .apprx.100-.apprx.320° by using N as the carrier gas. An exptl. investigation of the effects of the main components of the reaction mixture on $\langle \text{SYM115} \rangle$ (supplemented with some

literature data) revealed that the effects of N and propylene were

negligible and those of iso-PrOH, Me_2CO , and H pos. (the increase in $\langle \text{SYM115} \rangle$ being within one order). Kinetic investigations showed that a lower elec.-conductivity activation energy meant a lower reaction activation energy. The catalytic activity, x, (x = the yield of Me_2CO , %) and changes of $\langle \text{SYM115} \rangle$ in the reaction conditions, $\langle \text{SYM68} \rangle \log \langle \text{SYM115} \rangle$, agreed well for Ge and GaAs ($x_{\text{Ge}} > x_{\text{GaAs}}$ and $\langle \text{SYM68} \rangle$

$\log \langle \text{SYM115} \rangle_{\text{Ge}} > \langle \text{SYM68} \rangle \log \langle \text{SYM115} \rangle_{\text{GaAs}}$) but not for CuBr, apparently due

to its decomposition to elemental Cu in the reaction zone. Temperature dependences

of $\langle \text{SYM68} \rangle \log \langle \text{SYM115} \rangle$ and x were represented by couples of parallel straight lines. The relations between $\langle \text{SYM68} \rangle \log \langle \text{SYM115} \rangle$ and x were linear through the temperature range studied indicating thus that both quantities have the same determining factors (the extent of chemisorption is apparently related to the number of free electrons in the surface layer of the semiconductor catalyst).

L12 ANSWER 59 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Autoxidation of quinoline 1-oxide

AU Natsume, Sachiko; Itai, Takanobu

SO Chemical & Pharmaceutical Bulletin (1966), 14(5), 557-60

CODEN: CPBTAL; ISSN: 0009-2363

GI For diagram(s), see printed CA Issue.

AB Quinoline 1-oxide (I) on heating 9 hrs. at 70° with an equimolar amount tert-BuOK with bubbling of O yielded 3 kinds of compds. (in 41, 34, and 10% yields, resp.), viz. 1-hydroxycarbostryl (II), m. 190° (intense red ferric reaction; identity established by ethylation of II to 1-ethoxycarbostryl); 2,2'-biquinoline (III), m.p. and mixed m.p. (Nakano, CA 53, 16134a) 193°; and mono oxide (IV) of III, $\langle \text{SYM108} \rangle (\text{EtOH})$ 266, 334-336, shoulder 304 m $\langle \text{SYM109} \rangle$; $\langle \text{SYM108} \rangle (\text{dioxane})$

249, 273.5, 300-302, 331-333 m $\langle \text{SYM109} \rangle$. IV could be quant. transformed to III

after an absorption of an equimolar amount of H by catalytic hydrogenation and IV could be derived from III by partial oxidation with equimolar amount of monoperphthalic acid, accompanied with the simultaneous formation of 1,1'-dioxide (V) of III, m.

248-50°. In addition to II, III, and IV, carbostryl (VI) was detected (0.6%), accompanied by the recovery of 5% I. III, IV, VI, and I were separated by column chromatography of the basic fraction on Al_2O_3 , while

the acidic fraction mainly consisted of II. The above reaction was very sensitive to either the presence of O or the irradiation of visible light. When the reaction was carried out under sunlight or the irradiation of a 600-w. sun lamp, a fairly smooth reaction occurred, even without bubbling O, whereas in the dark, and without O, no reaction took place and 98% I was recovered. Moreover, when O was bubbled under irradiation of a sun lamp, 52% II was formed and 41% I was recovered, while under N atmospheric free

from O by passage through Fieser's solution, no reaction took place even with irradiation. Irradiation of uv light of $\langle \text{SYM108} \rangle$ 2537 Å. showed no appreciable effect on this reaction and the reaction was sufficiently inhibited by the addition of hydroquinone. The reaction proceeded less successfully both in the systems of ethanolic NaOEt and methanolic NaOMe , while in C_6H_6 or tetrahydrofuran solution in the presence of tert-BuOK, an exclusive formation of II was observed (73-92%). The reaction of some methylderivs. of quinoline 1-oxide was examined under similar conditions (first conditions). Following are given the quinoline 1-oxide used and the % of the resp. II, III, IV, VII, and quinoline 1-oxide carboxylic acid (VIII) along with other reaction products and recovery. Pyridine 1-oxide did not react in any way. The above exptl. results indicated that the reaction involved some radical intermediate rather than ionic. In fact, when di-tert-butyl peroxide was added to the reaction mixture under N atmospheric,

I gave the same products, viz. II, III, and IV. III, VI, V, and II were all recovered nearly quant. under the reaction conditions, and thus, all of them were unlikely to be possible intermediates.

L12 ANSWER 60 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Metalation of N,N-dimethylaniline

AU Lepley, Arthur R.; Khan, Wajid A.; Giumanini, Armida B.; Giumanini, Angelo

G.

SO Journal of Organic Chemistry (1966), 31(7), 2047-51

CODEN: JOCEAH; ISSN: 0022-3263

AB PhNMe₂ was metalated by refluxing with BuLi; o-Dimethylaminophenyl-tert-

carbinols were obtained when the metalation mixture was treated with ketones. Ketones with <SYM97> hydrogens gave carbinols which dehydrated under the reaction conditions producing the analogous conjugated olefins. The reaction of cyclohexene oxide with metalated PhNMe₂ gave predominantly the olefin identical with 1-(o-dimethylaminophenyl)cyclohexene from dehydration of 1-(o-dimethylaminophenyl)-1-cyclohexanol. The o- and m-dimethylaminophenylbis(trifluoromethyl)carbinols were formed from hexafluoroacetone in 71 and 19% yield, resp. These results parallel base-catalyzed H exchange data for PhNMe₂. The small amount, if any, of methyl group metalation seems to preclude participation of metalated PhNMe₂ in <SYM97>-alkylation reactions.

L12 ANSWER 61 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Catalytic synthesis of dimethylcyclopentadienes

AU Erivanskaya, L. A.; Hofman, H.; Shuikin, N. I.

SO Neftekimiya (1964), 4(4), 5304

CODEN: NEFTAH; ISSN: 0028-2421

AB Dimethylcyclopentadienes (I) were prepared by the catalytic dehydrogenation

of dimethylcyclopentenes (II). Starting materials were pure 1,2-dimethylcyclopentene (III), pure 2,4-dimethylcyclopentene (IV), and mixed II such as obtained by the catalytic dehydrogenation of methylcyclohexanols over Al₂O₃ with simultaneous ring contraction (CA 61, 6927h), including a fraction b737 91.5-92°, containing 84% IV, a fraction (V) b. 92-94°, containing 77% IV, and 3 fractions (VI) b. 80-105°. 1-Methylcyclopentene was treated with H₂O₂ and HCO₂H to give 50-5% 2-methylcyclopentanone (VII), b750 138.2°, d20 0.9194, n_D20 1.4352. 1,2-Dimethylcyclopentanol obtained from VII and MeMgI was oxidized with iodine to give 79% III, 13% 2,3-dimethylcyclopentene (VIII), and 8% putative 1-methyl-2-methylenecyclopentane. Fractionation gave 50% pure III, b740 103.5-4.5°, d20 0.7946, n_D20 1.4442. 4-Methylcyclopentanone was oxidized with HNO₈ to give <SYM98>-methyladipic acid, which was cyclized to

3-methylcyclopentanone. This ketone was converted as above into .apprx.56% IV, b744 92.4-2.6°, d20 0.7724, n_D20 1.4295, containing 1% 1,3-dimethylcyclopentene (IX). Dehydrogenation of the pure and mixed II was carried out in a flow-type apparatus at 600°/20-30 mm. and a space velocity of 1 hr.-l using a MoO₃-Al₂O₃ catalyst (X) except for one experiment

in which a CrO₃-K₂O-Al₂O₃ catalyst (XI) was used. After 1 hour reaction time, a 20-34% yield of I based on starting material and an .apprx.60-70% conversion yield was obtained; VI gave the lowest yield probably because of the presence of methylcyclohexenes and dimethylcyclopentanes. The catalyzates contained also 5-10% toluene and unconverted II, but the II separated from the catalyzates of IV and V contained 5-8% III not present in the starting material. Thus, under the reaction conditions, it may be preferable to use mixts. of II instead of pure II. Dehydrogenation of III over XI gave after 0.5 hr. 58% catalyzate containing 50% I and after a second 0.5-hr. period 85% catalyzate containing 43% I. The catalyzates were combined and a part was reduced with Raney Ni to a mixture of cis- and trans-1,2-dimethylcyclopentanes; another part was treated with Na and the Na derivative of dimethylcyclopentadiene was separated and decomposed with H₂O to

give 3.5 g. monomer, b130 53.5°, n_D20 1.4573, 1 g. dimer, b6 90-100°, n_D20 1.5050, and 3.5 g. resin. The adduct of the monomer with p-benzoquinone m. 88.5-89°. Chromatographic analysis showed that the catalyzates contained apparently 1,2- and 2,3-dimethylcyclopentadienes. Dehydrogenation of IV over X gave 10 g. catalyzate, which after dimerization gave 3.8 g. II, n_D20 1.4410, 1 g. dimer, n_D20 1.5164, and 1.3 g. residue. Thermal decomposition of the dimer gave a monomer (adduct with p-benzoquinone m. 70-3°). The II contained in the catalyzate consisted of 92% IV, 3% IX, and .apprx.5% III. Dehydrogenation of V over X gave 27 g. catalyzate of which 46% remained unchanged after dimerization. The fraction distilling at 100°, n_D20 1.4380, showed 66.5% IV, 21% IX, 6% VIII, and 8% III by gas chromatography. Dimerization gave 12% hydrocarbons, b80 40°, n_D20 1.4772, consisting mainly of II and toluene, 20% dimer, b6 85-98°, n_D20 1.5160, and 18% residue. Thermal decomposition of the dimer gave 3.5 g.

monomer (adduct with p-benzoquinone m. 83-5°) and an oil. After separation from the oil and repeated crystallization from isooctane, the adduct melted

at 89-9.5° and gave no m.p. depression with the adduct obtained

from the catalyzate of III.

L12 ANSWER 62 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Tritium labeling of natural products

AU Maurer, Rainer; Wenzel, Martin; Karlson, Peter

SO Nature (London, United Kingdom) (1964), 202(4935), 896-8

CODEN: NATUAS; ISSN: 0028-0836

AB A combination of the charcoal adsorption method (CA 59, 1954e, 4989c) with

Pt catalysis (Meshi and Takahashi, CA 58, 3064e) was used for tritium-labeling of natural products to obtain substantially higher specific activities and without a parallel increase in the radiochem. by-products. Thus, a solution of digitogenin (I) in C₆H₆-EtOH was

shaken with Pt-C catalyst [prepared by shaking a suspension of fine grained charcoal (particle size 0.1-0.3 mm.) in an aqueous solution of H₂PtCl₆.6H₂O in a

hydrogenator], the solvent removed so that an adsorption density of 6% resulted (22.6 mg. I on 355 mg. catalyst). The adsorption as well as the pure substance were enclosed in porous nylon bags; each sample sep. exposed to 2 c. tritium for 7.5 hrs. in an apparatus described by W., et al. (CA 55, 21681d). The adsorbed was I extracted from the catalyst by C₆H₆-EtOH

(1:1) at 85° (microsoxhlet; 100 min.) and tritium activity measured with a Packard Tricab liquid scintillation spectrometer (efficiency 28.2%); the amts. of substances were determined spectrophotometrically by means

of chromogen reaction (Walens, et al., CA 48, 7482c). The extracted was subjected to thin-layer chromatography using Kieselgel H as adsorbant, plates developed in cyclohexane-Me₂CO (1:1, volume/volume), sprayed with 5%

H₂SO₄, heated with a hair dryer, and finally spots developed with 1% vanillin-H₃PO₄ (50%). The cones bearing the radioactive I as disclosed by the color reaction and radioactive peak in the center chromatogram were carefully scraped from the plates, eluted with C₆H₆-EtOH, and rechromatographed. The characteristics of the tritiated I obtained were the same as for pure 25<SYM97>-I (yield 20-6% of the crude I to be tritiated); the product may still contain the 25<SYM98> isomer. The higher specific activities obtained with adsorbed substances are due either to the increased surface area under these reaction conditions or to a catalytic action of the carrier, or more probably to a combination of both.

L12 ANSWER 63 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Synthesis of <SYM97>- and <SYM103>-picoline by a vapor-phase catalytic reaction. I. Reaction products and the reaction conditions

AU Hatano, Takuya; Nakajima, Kazuo; Kurabayashi, Masahiro; Yanagiya, Koshin

SO Yuki Gosei Kagaku Kyokaiishi (1963), 21(9), 704-8

CODEN: YGKKAE; ISSN: 0037-9980

AB In order to carry out a simultaneous synthesis of <SYM97>- (I) and <SYM103>-picoline (II), a vapor-phase catalytic reaction of paraldehyde and NH₃ was carried out using silica-alumina catalyst. The products, besides I and II, contained a small amount of pyridine with traces of <SYM98>-picoline and EtNH₂. A large amount of high boiling pyridines, aldehyde condensation products, carbonaceous substances, and gaseous decomposition products was also formed. The reaction conditions were studied and it was found that the recycling of aldehyde raw materials was not favorable and deposition of carbonaceous substance on the catalyst caused rapid decrease in its selectivity to make it necessary to be regenerated frequently. The theoretical yield from aldehyde was 20 mole-% of I, 23 mole-% of II, 10 mole-% of high boiling pyridines at reaction temperature of 450° for 7 hrs. with 0.19 g. aldehyde/ml. catalyst/hr. space velocity and 200% excess (against paraldehyde) of NH₃.

L12 ANSWER 64 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

TI Naphtha hydroforming by irradiation

IN Folkins, Hillis O.

SO 2 pp.

AB The hydrocarbons are heated to their threshold thermal decomposition temperature (the

temperature at which 1% by weight of hydrocarbon decompose when subjected to the

temperature for 10 min. in the absence of catalyst), and while at this temperature are brought into contact with a solid, dehydrocyclization catalyst and simultaneously subjected to the emissions

from a radioactive source. H is mixed with the hydrocarbon charge in an

amount within the range of about 0.5 to 15 moles of H per mole of hydrocarbon. The pressure in the reaction zone may vary from about atmospheric to about 1000 lb./sq. in. or more. The high-energy radiations include <SYM103>-rays, neutrons, deuterons, hard x-rays, high-energy electrons, <SYM97>-particles, <SYM98>-particles, and the like. Energies of these radiations generally should be in the range of 0.4 to 20 m.e.v. or greater. As an example of the process, normal heptane is mixed with H in a mole ratio of 1 and passed through a fixed-bed catalyst consisting of molybdena on activated alumina, containing 9.5% molybdena, at 150 lb./sq. in. pressure and at 900°F., at a liquid hourly space velocity of 1. A 25% yield of toluene is obtained, and the gas make is 6%. Under the same reaction conditions, except that the reactor is exposed to radiation from a Co60 source having a radiation intensity of about 235,000 r./hr., a toluene yield of 35% is obtained, with a gas production of 6%.

L12 ANSWER 65 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
TI Kinetic equations for heptane reactions under catalytic reforming conditions

AU Feizkhanov, F. A.; Panchenkov, G. M.; Kolesnikov, I. M.
SO Neftekhimiya (1962), 2, 716-22

CODEN: NEFTAH; ISSN: 0028-2421

AB Several simultaneous or consecutive reactions take part in the catalytic reforming of n-heptane, including dehydrocyclization to toluene, isomerization, and hydrocracking of n-heptane or isoheptane. Three possible reaction schemes are suggested. For one of the proposed schemes, a detailed kinetic analysis is given, and the corresponding differential equations are derived. The equations cannot be integrated but allow a graphical treatment of exptl. data plotted in terms of conversion against the flow rate per g. of catalyst. By examination of the exptl. data, the authors found close agreement between the observed course of reaction and the reaction scheme, considering dehydrocyclization and isomerization as concurrent reactions and hydrocracking as consecutive to isomerization. Deviations from this scheme can, however, be expected for reaction conditions differing widely from those discussed. At 496° and 35 atmospheric, hydrocracking predominated; at 468°, isomerization predominated. The ratio of dehydrocyclization and isomerization rates is equal to the differential quotient dy/dz where y is the amount of toluene and z is the amount of isoheptane diminished by the amount of hydrocracked products. Thus, at least the selectivity of catalyst action can be evaluated in a simple way.

L12 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
TI Organosilicon compounds. XXVIII. Direct synthesis of ethylchlorosilanes
AU Bazant, V.; Kraus, M.

SO Collection of Czechoslovak Chemical Communications (1961), 26, 2028-34
CODEN: CCCCAK; ISSN: 0010-0765

AB cf. CA 55, 24543d. Kinetic studies of the Cu-catalyzed reaction of EtCl with Si at 200-320° carried out by the method of Darby and Kembal (CA 52, 7121f) revealed that all ethylchlorosilanes (I) arise by parallel reactions. The direct synthesis of I by means of EtCl is considerably less selective than with MeCl. This selectivity decreases with rising temperature. Formation of EtHSiCl₂ is a primary reaction which competes (after the adsorption of EtCl on the contact mass) with the formation of the other I. This excludes the notion that EtCl primarily decompose to C₂H₄ and HCl, which then enter the reaction together with EtCl and Si, since addition of HCl to EtCl does not affect the conversion of EtCl to EtHSiCl₂, although the content of EtSiCl₃ and SiCl₄ in the product is raised. The influence of the reaction conditions on the course of the reactions is studied. With decreasing partial pressure of EtCl the formation rate of I falls more steeply than that of C₂H₄. The reaction mechanism is discussed.

L12 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
TI Reactor and regenerator for fluid catalytic cracking
IN Rehbein, Charles A.

AB A process and apparatus are described for the conversion of hydrocarbons and the simultaneous regeneration of the fouled fluidized catalyst. The reactant vapors are continuously passed with finely divided catalyst into the bottom of a reactor maintained in a fluidized state and under reaction conditions. The spent catalyst is continuously withdrawn from the top of the fluidized bed by overflow over a weir which is located at the mid-point of the reactor, directly into a standpipe. A stripping gas is continuously introduced into the standpipe to regenerate the catalyst, and the upper level of the

spent catalyst in the standpipe is maintained below the level of fluidized bed. The finely divided catalyst overflows into the standpipe at a rate which is independent of the rate of withdrawal of the catalyst from the bottom of the standpipe.

L12 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
TI Aluminum halide-olefinic ketone complexes as catalyst for hydrocarbon reactions

IN Pines, Herman

AB A new catalyst for alkylation, isomerization, autodestructive alkylation, and dealkylation consists of the addition compound of Al halide and an unsatd.

ketone in the mol. ratio of about 1:1. The ratio can be increased to 3:1 but higher ratios no longer show the advantages of the special catalyst. Depending on the mol. weight of the ketone, the catalysts are liquids or solids; ketones of less than 10 C atoms give liquid complexes. The Al halide-olefinic ketonates do not form substantial amts. of sludge in reactions involving olefins and aromatics and do not cause cracking when used for the alkylation of an isoparaffin with an olefin. The most desirable catalyst consists of equal mols. of AlCl₃ and mesityl oxide. The catalyst is especially suited for the isomerization of alkyl naphthenes to compds. with an increased or decreased number of C atoms in the ring, dependent on the hydrocarbon and the reaction conditions. Methylcyclohexane, e.g., can be isomerized to dimethylcyclopentane or ethylcyclopentane. Methylcyclopentane can be isomerized to cyclohexane which can be hydrogenated to C₆H₆ and this reaction is capable of general application. The catalyst can also be used for the dealkylation of aromatics having side chains of at least 4 C atoms. Autodestructive alkylation in the presence of this catalyst leads by simultaneous cracking and alkylation of the paraffin or naphthene charged to a product of wider boiling range than the starting material. Alkylation with this catalyst is carried out at 10-70° under otherwise normal com. alkylation conditions. In an example for autodestructive alkylation, 2.2 mols. n-C₅H₁₂ was stirred 2 hrs. at 10-25° with a mixture of 0.5 mol. mesityl oxide and 0.67 mol. AlCl₃. After separation of the catalyst by decantation the yield of hydrocarbons amounted to 89% (based on C₅H₁₂ charged) and consisted of 12% iso-C₄H₁₀, 11.5% iso-C₅H₁₂, 61.5% n-C₅H₁₂, and 8% C₆H₁₄ and C₇H₁₆. Alkylation of aromatics is illustrated by an experiment in which 40 g. anhydrous AlCl₃ and 30 g. mesityl oxide were cooled separately to -78° and subsequently mixed under cooling. The solid reaction product (20 g.) was mixed with 35 g. C₆H₆ and 15 g. tert-BuCl and allowed to stand at 25° 2 hrs. The reaction product (40 g. liquid) contained 8 g. tert-BuPh and 8.5 g. higher alkylbenzenes, mainly p-(tert-Bu)₂C₆H₄.

L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of Acinetobacter sp. YQ231

AU Zhao, Yuqiao; Xu, Jianhe

SO Cuihua Xuebao (2003), 24(8), 613-618

CODEN: THHPD3; ISSN: 0253-9837

AB The effects of reaction conditions on the reaction rate and selectivity of the enantioselective hydrolysis of racemic 4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone (HMPC) acetate

by Acinetobacter sp. strain YQ231 were investigated. The apparent activity of the resting cells increases with pH up to 11.0, but the non-selective simultaneous hydrolysis of the chiral ester becomes significant at pH>9.0. Therefore, to prevent possible non-enzymic hydrolysis of the ester and possible racemization of the product, the enzymic resolution is carried out at pH 8.0. When the cells are preserved in buffers at pH ranging from 9.0 to 10.5 for 12 h, the residual activity of the resting cells increases. This is attributed to the possible permeabilizing effect on the cell membrane, which facilitates the trans-membrane transport of substrates and products. The highest activity of the cells is observed at 50°, and the best stability at 30°. Nonyl phenol polyethyleneoxy ether is the most suitable emulsifier for the substrate and its optimal concentration is 15 g/L in regarding to the enantioselectivity of the esterase-catalyzed reaction. The enzymic reaction is inhibited by the product HMPC, but not by the substrate HMPC acetate up to 1.0 mol/L. The esterase in the resting cells preferentially hydrolyzes the (R)-enantiomer of the racemic ester, producing enantiopure (R)-HMPC. The enantiomeric ratio (E-value) is 50 in the case of 250 mmol/L substrate.

- L6 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Scalability of Microwave-Assisted Organic Synthesis. From Single-Mode to Multimode Parallel Batch Reactors
 AU Stadler, Alexander; Yousefi, Behrooz H.; Dallinger, Doris; Walla, Peter; Van Der Eycken, Erik; Kaval, Nadya; Kappe, C. Oliver
 SO Organic Process Research & Development (2003), 7(5), 707-716
 CODEN: OPRDFK; ISSN: 1083-6160
 AB The direct scalability of microwave-assisted organic synthesis (MAOS) in a prototype laboratory-scale multimode microwave batch reactor is investigated. Several different organic reactions have been scaled-up typically from 1 mmol to 100 mmol scale. The transformations include multicomponent chemistries (Biginelli dihydropyrimidine and Kindler thioamide synthesis), transition metal-catalyzed carbon-carbon cross-coupling protocols (Heck and Negishi reactions), solid-phase organic synthesis, and Diels-Alder cycloaddn. reactions using gaseous reagents in pre-pressurized reaction vessels. A range of different solvents (high and low microwave absorbing), Pd catalysts (homogeneous and heterogeneous), and varying reaction times and temps. have been explored in these investigations. In all cases, it was possible to achieve similar isolated product yields on going from a small scale (ca. 5 mL processing volume) to a larger scale (max 500 mL volume) without changing the previously optimized reaction conditions (direct scalability). The prototype, bench top multimode microwave reactor used in the present study allows parallel processing in either quartz or PTFE-TFM vessels with maximum operating limits of 300 °C and 80 bar of pressure. The system features magnetic stirring in all vessels, complete online monitoring of temperature, pressure and microwave power, and the ability to maintain inert or reactive gas atmospheric
- L6 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Microwave assisted reactions with arylboronic acids
 AU Gupta, Varsha
 SO Abstracts, 31st Northeast Regional Meeting of the American Chemical Society, Saratoga Springs, NY, United States, June 15-18 (2003), 171
 Publisher: American Chemical Society, Washington, D. C.
 CODEN: 69EBFV
 AB We have been interested in constructing three- and four-component condensation reaction libraries to create diverse small mol. drug like compds. for rapid lead generation. These multicomponent condensations often require long reaction times and rigorous purifications. Microwave technol. has provided a novel tool to rapidly optimize and generate such libraries in parallel fashion. A strategy for the generation of boronic acid imine arylation library using microwave will be presented. Despite extensive research in palladium catalyzed bi-aryl synthesis, Suzuki coupling with 4-chloroindole using conventional reaction conditions yields 4-arylindole in poor yields. A microwave assisted palladium catalyzed synthesis of 4-arylindoles will be presented.
- L6 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Optimization of reaction conditions and stabilization of phenylalanine ammonia lyase-containing Rhodotorula glutinis cells during bioconversion of trans-cinnamic acid to L-phenylalanine
 AU El-Batal, Ahmed I.
 SO Acta Microbiologica Polonica (2002), 51(2), 139-152
 CODEN: AMPOAX; ISSN: 0137-1320
 AB Studies were performed to elucidate the optimal reaction conditions (pH, temperature, ammonia concentration and biocatalyst loading) for bioconversion of trans-cinnamic acid (t-CA) to L-phenylalanine (L-Phe) by L-phenylalanine ammonia lyase (PAL) containing Rhodotorula glutinis cells. All treatments with permeabilizing agents stimulated L-Phe production and also enhanced instability of the catalyst, except Triton X-100 which gave a superior (56%) increase in conversion as compared to the control and a significant stabilization of PAL enzyme. Inclusion of several activity modifiers and stabilizer additives in reaction mixts. were shown to enhance the yield of L-Phe and maintained PAL stability over several successive incubations during the bioconversion process. Maximum stabilization of PAL and enhancement of L-Phe production was achieved with addition of 20% polyhydric alc. (glycerol). The production of L-Phe continued to the fifth cycle and the total yidd increased 2.3 times compared to the yield produced by the control (without glycerol addition) during the repeated batch process. Reducing agents such as 2-mercaptoethanol and thioglycolic acid were added to the bioconversion mixture in order to reduce the effects of oxygen on PAL catalyst
- life. Production of L-Phe by addition of 400 mgL-1 of thioglycolic acid was maximized over the control by 55%. When both 20% glycerol and 400 mgL-1 thioglycolic acid were simultaneously present in the reaction mixture, reuseability and stability of biocatalyst (PAL) were extended to eight consecutive cycles and conversion rate and overall productivity of L-Phe were higher than that of the control. These results may lead to improvements in the production of the essential amino acid L-Phe.
- L6 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Parallel catalyst screening instrumentation
 AU Andrews, Kara; Hsiao, Gregor
 SO Chimica Oggi (2001), 19(3/4), 53-55
 CODEN: CHOGDS; ISSN: 0392-839X
 AB A well-designed parallel pressure reactor system which employs multiple small scale reactors can be employed to optimize catalytic reactions such as hydrogenation, carbonylation, and olefin polymerization. Proper implementation of parallel technol. results in a cost effective compact unit which increases the efficiency and still allows sufficient flexibility for difficult research, yielding accurate and reliable data for the evaluation of appropriate catalytic reaction conditions.
- L6 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Removal of ammonia and phenol by using hydrophobic catalyst
 AU Huang, Tung-Li; Sheu, Shib-Hsiung
 SO Shiyu Jikan (2001), 37(1), 17-27
 CODEN: SYCKE4; ISSN: 1022-9671
 AB The streams of ammonia and phenol containing wastewaters produced in petrochem. refineries are usually characterized by high concentration and high temperature, and are not treatable by biol. methods directly. A chemical or phys. pretreatment is required before subsequent biol. processing. In this study, a combined process of stripping and catalytic oxidation to remove ammonia and phenol from water has been successfully developed using a hydrophobic catalyst. The initial feasibility study was done in a batch reactor. Ammonia and phenol were converted to N₂, CO₂ and H₂O under a mild reaction condition of 120°C and partial pressure of 0.3 MPa. Both stripping and catalytic oxidation by using hydrophobic Pt/styrene divinyl benzene copolymer (SDB) catalyst were carried out simultaneously in a single trickle-bed reactor, possessing a high removal rate and long reaction time in comparison with that using hydrophilic Pt/SYM103-Al₂O₃ catalyst. Small amts. of nitrites and nitrates were detected in the resultant reaction solution, resulting from the aqueous absorption of gaseous nitrogen oxides. A statistically based exptl. design method, Two-Level Factorial Design (TEFD), was applied to identify the critical factors that affect process efficiency and to uncover the interaction between the factors. The results showed that temperature, PO₂ and the presence of phenol are the critical factors, and the presence of phenol adversely affects the temperature dependence of the ammonia oxidation. The statistically based exptl. design is a powerful tool to more quickly identify the key factors affecting the process and to understand the interactions between factors. Once these critical elements have been determined, optimizing the process performance can be approached effectively.
- L6 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI 6,6-Dimethylhept-1-en-4-yn-3-ol: a useful model for investigation of the effect of trifluoroacetic acid on the stereoselectivity of allylic rearrangement
 AU Faigl, Ferenc; Barcza, Tibor; Agai, Bela; Toke, Laszlo
 SO ACH - Models in Chemistry (1999), 136(5-6), 593-598
 CODEN: ACMCEI; ISSN: 1217-8969
 AB Reactions of 6,6-dimethylhept-1-en-4-yn-3-ol with an excess of trifluoroacetic acid or equivalent amount of trifluoroacetic anhydride have effected simultaneous acylation and allylic rearrangement providing (E)-6,6-dimethylhept-2-en-4-yn-1-ol trifluoroacetate with excellent stereoselectivities and yields. Systematic investigation of the product distribution as a function of the molar ratio and the reaction time was carried out for optimization of the reaction conditions.
- L6 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Investigation of conditions in porphyrin-forming reactions using an automated chemistry workstation
 AU Riggs, Jennifer A.; Wagner, Richard W.; Li, Feirong; Du, Hai; Lindsey,

- Jonathan S.
- SO Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25 (1999), INOR-113 Publisher: American Chemical Society, Washington, D. C.
CODEN: 67GHA6
- AB Optimization of reaction conditions, a tedious but integral part of all facets of synthetic chemical, can be performed rapidly and efficiently with new automated workstations. We have designed and constructed an automated microscale chemical workstation capable of parallel and/or adaptive experimentation. We are applying this system toward the optimization of various porphyrin-forming reactions. As one example, we have explored cocatalysis conditions for a high concentration synthesis of meso-tetramesitylporphyrin (TMP). As the concns. of mesitaldehyde and pyrrole increase from 10-100 mM, optimal yields of TMP are obtained with a commensurate increase in BF₃-etherate but with constant amts. of ethanol. We are currently examining other catalytic, cocatalytic, and general reaction conditions for a variety of substrates in porphyrin-forming reactions.
- L6 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI Factors which affect the catalytic activity of iron(III) meso-tetrakis(2,6-dichlorophenyl)porphyrin chloride in homogeneous system
AU Iamamoto, Yassuko; Assis, Marilda D.; Ciuffi, Katia J.; Sacco, Herica C.; Iwamoto, Lidia; Melo, Andrea J. B.; Nascimento, Otaciro R.; Prado, Cynthia M. C.
SO Journal of Molecular Catalysis A: Chemical (1996), 109(3), 189-200
CODEN: JMCCF2; ISSN: 1381-1169
- AB An optimization study of the reaction conditions of Fe(TDCPP)Cl when it is used as catalyst in the hydroxylation of cyclohexane by iodosylbenzene (PhIO) has been carried out. It was found that Fe(TDCPP)Cl follows the classical PhIO mechanism described for Fe(TPP)Cl, which involves the monomeric active species FeIV(O)P+<SYM183> (I). In the optimized condition [Fe(TDCPP)] = 3.0 + 10-4 mol l-1 in 1,2-dichloroethane (DCE); ultrasound stirring of 0°C; PhIO/FeP molar ratio = 100], this FeP led to a yield of cyclohexanol (C-ol) of 96% and a turnover number of 96. Therefore, Fe(TDCPP)Cl may be considered a good biomimetic model and a very stable, resistant and selective catalyst, which yields C-ol as the sole product. DCE showed to be a better solvent than dichloromethane (DCM), 1 DCE:1 MeOH mixture or acetonitrile (ACN).
Since the FeIV(O)P+<SYM183> is capable of abstracting hydrogen atom from DCM, MeOH or ACN, the solvent competes with the substrate. Presence of O₂ lowers the yield of C-ol, as it can further oxidize this alc. to carboxylic acid in the presence of radicals. Presence of H₂O also causes a decrease in the yield, since it converts the active species I into FeIV(OH)P, which cannot oxidize cyclohexane. Addition of excess imidazole or OH- to the system results in a decrease in the yield of C-ol, due to the formation of the hexacoordinated complexes Fe(TDCPP)Im₂+ (low-spin, <SYM98> 2 = 2.5 + 108 mol-2 l2) and Fe(TDCPP)(OH)₂- (high-spin, <SYM98> 2 = 6.3 + 107 mol-2 l2). The formation of both Fe(TDCPP)Im₂+ and Fe(TDCPP)(OH)₂- complexes were confirmed by EPR studies. The catalytic activities of Fe(TDCPP)Cl and Fe(TFPP)Cl were compared. The unusually high yields of C-ol with Fe(TFPP)Cl obtained when ultrasound, DCM and O₂ atmospheric were used, suggest that a parallel mechanism involving the <SYM109>-oxo dimer form, O₂ and radicals may also be occurring with this FeP, besides the PhIO mechanism.
- L6 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI The diffusion model of solid-state catalytic hydrogen isotope exchange. Isoradiochemical purity dependencies of the exchange level on temperature for thymine
AU Filikov, A. V.
SO Synth. Appl. Isot. Labelled Compd. 1991, Proc. Int. Symp., 4th (1992), Meeting Date 1991, 375-82. Editor(s): Buncel, Erwin; Kabalka, George Walter. Publisher: Elsevier, Amsterdam, Neth.
CODEN: 58MNAG
- AB An approach to using the diffusion model theory for reaction condition optimization is presented. Practical application of solid-state catalytic isotope exchange (SSCIE) for production of tritium-labeled organic compds. requires selecting the reaction temperature and time to ensure the maximum molar radioactivity of the compound for a preset level of byproduct yield. Theor. molar radioactivity dependencies of isotope-substituted thymine on reaction temperature have been calculated for a number of radiochem. purities (91-99%). Previously exptl. obtained consts. for thymine SSCIE reactions (isotope exchange with parallel hydration of thymine) have been used.
- L6 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI Catalytic addition of formaldehyde to unsaturated oleochemicals
AU Behr, A.; Handwerk, H. P.
SO Fett Wissenschaft Technologie (1992), 94(12), 4437
CODEN: FWTEEG; ISSN: 0931-5985
- AB Catalytic reactions of CH₂O with Me oleate (I) yielded 1:1, 1:2 (main product), and 4:1 addition compds. as well as dihydrofuran and dihydropyran structures formed by intramol. dehydration of 2:1 products. A mechanism for the catalysis with SnCl₄ is given. Results from a catalysts screening showed that product yield depended on the catalysts concentration; standard expts. were performed with a ratio of 20:1 for which e.g. a 74% yield was achieved applying H₂PtCl₆ (82% for an increased catalysts concentration of 10:1). A 20-40% yield was already observed at approx. 30° with the catalysts RuCl₃, H₂PtCl₆, and SnCl₄, however optimum yields were achieved at 70-90° in propylene carbonate as optimum solvent and a 2-fold surplus of CH₂O. Complete conversion of I was already observed after 30 min with the latter catalysts. Exemplary results are also presented from CH₂O addition to other fatty acid Me esters (e.g. undecenoate) which showed simultaneous reaction of double bonds located inside or at the end of the chain.
- L6 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI Substitution catalytic hydrogenation of C2 chloro derivatives
AU Zaidman, O. A.; Verkhutova, E. I.; Zhanaveskin, L. N.; Treger, Yu. A.
SO Khimicheskaya Promyshlennost (Moscow, Russian Federation) (1991), (9), 517-22
CODEN: KPRMAW; ISSN: 0023-110X
- AB The selectivity of the Pd-catalyzed substitution hydrogenation of the chloroethanes (CE) CH₂ClCH₂Cl, CH₂ClCHCl₂, MeCCl₃, and CHCl₂CHCl₂, as well as 1:1 mixts. of cis- and trans-1,2-dichloroethenes, at 200-350° was studied as a function of reaction temperature (T), reactant ratio, contact time (t), and catalyst composition in order to optimize the conversion of these typical waste byproducts of organochlorine compound manufacture to useful products.
Conversion of CE, with the exception of MeCCl₃, over 0.5% Pd/Al₂O₃ catalyst gave C₂H₆ and C₂H₄ as the main products, with unsatd. compound yield increasing with increasing T. Increasing the CE-H mol ratio in the reaction mixture by a factor of 4 significantly increased the unsatd. product yield in the conversion, although the degree of CE conversion simultaneously decreased. Increasing t from 3 to 18 s increased the degree of CE conversion, but product composition remained unchanged. In dichloroethene (I) conversion, the highest selectivity for vinyl chloride (II) combined with a satisfactory degree of I conversion was obtained with Pd/KSK silica gel catalyst with sp. surface 30 m²/g. Optimum I conversion conditions (T 200°, t 8-10 s, H-I mol ratio 1.05, Pd content in catalyst 0.1%) gave I conversion 42% and product of composition II 81, MeCH₂Cl 3, CH₂ClCH₂Cl 6.5, C₂H₆ 4.5 and C₂H₄ 5%.
- L6 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
TI Ethylene from natural gas by direct catalytic oxidation
AU Geerts, J. W. M. H.; Van Kasteren, J. M. N.; Van der Wiele, K.
SO Comm. Eur. Communities, [Rep.] EUR (1991), EUR 13061, 125 pp.
CODEN: CECE99; ISSN: 0303-755X
- AB The title report describes optimizing the phys. parameters of the oxidative coupling catalyst, defining the optimum reactor design and reaction conditions, collecting data for modeling of the chemical reaction, and process design and economic evaluations. Li-doped MgO catalyst was optimized with respect to catalytic performance. Essential for the catalytic activity and selectivity is the presence of Li. The most suitable reactor was fluidized bed reactor because of the high exothermicity of the reaction. The optimum reaction conditions for reaching the maximum ethylene yield (18%) for the longest time were 800°/1 atmospheric using a CH₄/O = 5 ratio gas-feed mixture at 0.6 g-s/mL catalyst. The reaction mechanism was described as a complicated mixture of heterogeneous (catalytic

-) and homogeneous (gas phase) reactions occurring simultaneously . Coupling to ethane takes place in the gas phase. Ethane is dehydrogenated on the catalyst or in the gas phase to ethylene, which in turn gets easily oxidized into CO and CO₂ which are mainly formed at the catalyst surface. A computer program was developed which simulated the network reaction (>150 elementary radical reactions) of the homogeneous gas phase.
- L6 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Methane steam reforming: II. Diffusional limitations and reactor simulation
 AU Xu, Jianguo; Froment, Gilbert F.
 SO AIChE Journal (1989), 35(1), 97-103
 CODEN: AICEAC; ISSN: 0001-1541
- AB Given the intrinsic kinetics, the tortuosity factor of a Ni/MgAl₂O₄ catalyst was determined under reaction conditions by minimizing the sum of squares of residuals of the exptl. and the simulated conversions. The parallel crosslinked pore model with uncorrelated pore size distribution and orientation was used in the calcn. of the effective diffusivities. A modified collocation method was used to obtain the partial pressure profiles of the reacting components in the catalyst pellet. The simulation of the exptl. reactor during the optimization of the tortuosity factor also yielded the effectiveness factors of the reactions. The results of the simulation of an industrial steam reformer are also discussed.
- L16 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane
 AU Wang, Haihui; You, Cong; Yang, Weishen
 SO Catalysis Letters (2002), 84(1-2), 101-106
 CODEN: CALEER; ISSN: 1011-372X
- AB An oxygen permeable mixed ion and electron conducting membrane (OPMIECM) was used as an oxygen transfer medium as well as a catalyst for the oxidative dehydrogenation of ethane to produce ethylene. O₂- species transported through the membrane reacted with ethane to produce ethylene before it recombined to gaseous O₂, so that the deep oxidation of the products was greatly suppressed. As a result, 80% selectivity of ethylene at 84% ethane conversion was achieved, whereas 53.7% ethylene selectivity was obtained using a conventional fixed-bed reactor under the same reaction conditions with the same catalyst at 800 °C. A 100 h continuous operation of this process was carried out and the result indicates the feasibility for practical applications.
- L16 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI n-Hexane oxyfunctionalization by hydrogen peroxide over titanium silicalite containing catalytic membranes
 AU Wu, S. Q.; Bouchard, C.; Kaliaguine, S.
 SO Proceedings of the International Zeolite Conference, 12th, Baltimore, July 5-10, 1998 (1999), Meeting Date 1998, Volume 2, 1399-1402. Editor(s): Treacy, M. M. J. Publisher: Materials Research Society, Warrendale, Pa. CODEN: 68DCAH
- AB The concept of catalytic membrane used as interphase contactor is illustrated with the example of oxyfunctionalization of n-hexane by aqueous H₂O₂ using composite membranes in which titanium silicalite (TS-1) is embedded in a polydimethylsiloxane (PDMS) matrix. The best advantage of using this catalytic membrane interphase contactor is to avoid the use of a co-solvent in the biphasic reaction medium. The exptl. results show that under typical reaction conditions it is possible to obtain reaction rates per unit mass of catalyst that are of same order of magnitude than in the conventional batch reactor with suspended catalyst. The rates and selectivity to n-hexanol can even be improved by introducing hydrophilic functional groups in the polymer matrix. The series of results demonstrate the great potential of these catalytic membranes for com. application, since the concept is potentially applicable and essentially beneficial for any multiphase reactions. A kinetic permeation-reaction model was established in this study to predict the reactant concentration profiles and the average reaction rates within the various catalytic membranes examined. The calcn. results fit well the results obtained in the expts.
- L16 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Catalytic performance of an ultrafine Cu/ZnO/Al₂O₃ catalyst prepared by gel-oxalate coprecipitation
- AU Wu, Xiaohui; Liu, Jinyao; Qiu, Xianqing; Liang, Yu; Zheng, Zhi; Liu, Chongwei; Zhu, Qiming
 SO Tianranqi Huagong (1999), 24(1), 20-23
 CODEN: THTKEF; ISSN: 1001-9219
- AB Activity of an ultrafine Cu/ZnO/Al₂O₃ catalyst prepared by gel-oxalate copptn. (GOCP) is evaluated at different temps. and space velocities for methanol synthesis. The spacetime yield of methanol reaches 0.49 g/g cat<SYM183>h by using the ultrafine catalyst at 2.0 MPa, 6000 h⁻¹ and 230°, higher than that by using overseas ICI-51-3 and BASF catalysts in the same reactor under the same reaction conditions. The x-ray diffraction and TEM results show that they are different in structure.
- L16 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Application of Cu-Pd composite membranes in dehydrogenation of methanol to methyl formate
 AU Mo, Xunhua; Lu, Guanzhong; Yan, Jingfeng; Wang, Junsong
 SO Cuihua Xuebao (1998), 19(1), 14-17
 CODEN: THHPD3; ISSN: 0253-9837
- AB Dehydrogenation of methanol to Me formate (MeF) in Cu and Cu-Pd catalytic membrane reactors (CMR) at atmospheric pressure was studied. For the title reaction, the Cu composite catalytic membrane reactor prepared by ion exchange method exhibits better performance than the fixed-bed reactor (FBR) under the same reaction conditions. At 240°, the conversion of MeOH and yield of MeF are 57.3% and 50.0% in CMR, while in FBR, 43.1% and 36.9%, resp. The Cu-Pd composite membrane behaves two functions of catalysis for the title reaction and permselectivity for hydrogen at the same time, but its catalytic activity for dehydrogenation of MeOH is lower than that of Cu composite CMR. Some impact parameters on preparation of membranes have also been investigated.
- L16 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Synthesis of dimethyl ether and alternative fuels in the liquid phase from coal-derived synthesis gas: Task 3.2: Screen novel catalyst systems; Task 3.3: Evaluation of the preferred catalyst system
 AU Underwood, R. P.
 SO Report (1993), DOE/PC/89865-T7; Order No. DE93013075, 77 pp. Avail.: NTIS
 From: Energy Res. Abstr. 1993, 18(9), Abstr. No. 25531
- AB The exptl. investigations, which involved bench-scale reactor studies, focused primarily on three areas: (1) one-step, slurry-phase syngas conversion to hydrocarbons or methanol/hydrocarbon mixts. using a mixture of methanol synthesis catalyst and methanol conversion catalyst in the same slurry reactor; (2) slurry-phase conversion of syngas to mixed alcs. using various catalysts; and (3) one-step, slurry-phase syngas conversion to mixed ethers using a mixture of mixed alcs. synthesis catalyst and dehydration catalyst in the same slurry reactor. The exptl. results indicate that, of the three types of processes investigated, slurry phase conversion of syngas to mixed alcs. shows the most promise for further process development. Evaluations of various mixed alcs. catalysts show that a cerium-promoted Cu/ZnO/Al₂O₃ methanol synthesis catalyst has the highest performance in terms of rate and selectivity for C₂+ alcs. In fact, once-through conversion at industrially practical reaction conditions yielded a mixed alcs. product potentially suitable for direct gasoline blending. Moreover, an addnl. attractive aspect of this catalyst is its high selectivity for branched alcs., potential precursors to isoolefins for use in etherification.
- L16 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
 TI Poly- or copolymerization of ethylene by gas phase method by using a fluidized bed reactor
 SO Jpn. Kokai Tokkyo Koho, 17 pp.
 CODEN: JKXXAF
- AB A method was described for continuously manufacturing an ethylene homo- or copolymer with another <SYM97>olefin in the substantial absence of aqueous liquid media by using a catalyst comprising a supported-type halogenated transition metal solid component and an organometallic compound, and by using a multistage reactor comprising a plurality of fluidized bed

- reactors. A polymer size screening region was provided. The polymer yield was adjusted to $< \text{SYM163} > 30,000$ times the amount of solid catalyst component used in each stage (except the last stage reactor) if the polymer d. was $< 0.945 \text{ g/cm}^3$ or $< 15,000$ times if the d. was $< \text{SYM179} > 0.945 \text{ g/cm}^3$. The polymer yield was adjusted throughout all the stages to > 5000 times the amount of solid catalyst component. A catalyst was used which satisfied the equation $(t_1/t_2) < 2$ [where t_1 and t_2 represent the time required to produce (resp.) 30,000 and 40,000 times the amount of polymer of the supported-type of halogenated transition metal solid component when the same polymerization test was carried out under the reaction conditions of the 1st reactor] and when the polymer d. was $< 0.945 \text{ g/cm}^3$; or $(t_3/t_4) < 2$ (where t_3 and t_4 represent the time required to produce 15,000 and 20,000 times the amount of polymer, resp.) when the polymer d. was $< \text{SYM179} > 0.945 \text{ g/cm}^3$. For example, 1-butene-ethylene copolymer [901929-8] having a wide mol. weight distribution and excellent moldability was produced.

L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

TI Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane

AU Wang, Haihui; You, Cong; Yang, Weishen

SO Catalysis Letters (2002), 84(1-2), 101-106

CODEN: CALEER; ISSN: 1011-372X

AB An oxygen permeable mixed ion and electron conducting membrane (OPMIECM)

was used as an oxygen transfer medium as well as a catalyst for the oxidative dehydrogenation of ethane to produce ethylene. O_2 -species transported through the membrane reacted with ethane to produce ethylene before it recombined to gaseous O_2 , so that the deep oxidation of the products was greatly suppressed. As a result, 80% selectivity of ethylene at 84% ethane conversion was achieved, whereas 53.7% ethylene selectivity was obtained using a conventional fixed-bed reactor under the same reaction conditions with the same catalyst at 800 °C. A 100 h continuous operation of this process was carried out and the result indicates the feasibility for practical applications.

L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

TI Application of Cu-Pd composite membranes in dehydrogenation of methanol to methyl formate

AU Mo, Xunhua; Lu, Guanzhong; Yan, Jingfeng; Wang, Junsong

SO Cuihua Xuebao (1998), 19(1), 14-17

CODEN: THHPD3; ISSN: 0253-9837

AB Dehydrogenation of methanol to Me formate (MeF) in Cu and Cu-Pd catalytic

membrane reactors (CMR) at atmospheric pressure was studied. For the title reaction, the Cu composite catalytic membrane reactor prepared by ion exchange method exhibits better performance than the fixed-bed reactor (FBR) under the same reaction conditions. At 240°, the conversion of MeOH and yield of MeF are 57.3% and 50.0% in CMR, while in FBR, 43.1% and 36.9%, resp. The Cu-Pd composite membrane behaves two functions of catalysis for the title reaction and permselectivity for hydrogen at the same time, but its catalytic activity for dehydrogenation of MeOH is lower than that of Cu composite CMR. Some impact parameters on preparation of membranes have also been investigated.

L18 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

TI A comparison of the fixed-bed, liquid-phase ("slurry") and fluidized-bed techniques in the Fischer-Tropsch synthesis

AU Hall, C. C.; Gall, D.; Smith, S. L.

SO Journal of the Institute of Petroleum (1952), 38, 84576

CODEN: JIPEA6; ISSN: 0020-3068

AB Synthesis expts. were made with fused and sintered Fe catalysts in laboratory-scale, fixed-bed, liquid-phase (slurry), and fluidized-bed reactors under similar reaction conditions. The following conclusions were made. By allowing for the increase in activity which accompanies reduction in particle size of fused and sintered Fe catalysts, the reaction rate in a fixed bed is the same as or somewhat greater than that in a fluidized bed, but in a slurry system the rate is appreciably less. The space-time yield is potentially greater in the fixed bed and lower in the liquid phase, but in practice the higher space-time yield would be obtained in a fluidized bed. Selectivity is approx. the same in the fixed and fluid beds, but is appreciably higher in the slurry system, owing to direct contact between

catalyst particles and liquid medium, preventing local high temps. The boiling range and olefin contents of the liquid products are independent of the synthesis technique. With a particular catalyst and reaction temperature C formation is controlled by the partial pressure of H in the total reactor feed. The rate of the synthesis reaction is a linear function of operating pressure over the range of 300-675 lb./sq. in. in all 3 processes. The synthesis-gas space velocity (time of contact of the gas in the reaction zone) exerts a greater control over the reaction rate than the gas throughput per unit weight of catalyst. The activity of the catalyst increases with a decrease of its concentration in the reaction zone. There appears to be possibilities of increasing the practical spacetime yield by the fixed-bed technique, and of increasing the selectivity of the fluid-bed process, but maximum selectivity and flexibility will probably always be obtained in a liquid-phase system.

L24 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

TI Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane

AU Wang, Haihui; You, Cong; Yang, Weishen

SO Catalysis Letters (2002), 84(1-2), 101-106

CODEN: CALEER; ISSN: 1011-372X

AB An oxygen permeable mixed ion and electron conducting membrane (OPMIECM)

was used as an oxygen transfer medium as well as a catalyst for the oxidative dehydrogenation of ethane to produce ethylene. O_2 -species transported through the membrane reacted with ethane to produce ethylene before it recombined to gaseous O_2 , so that the deep oxidation of the products was greatly suppressed. As a result, 80% selectivity of ethylene at 84% ethane conversion was achieved, whereas 53.7% ethylene selectivity was obtained using a conventional fixed-bed reactor under the same reaction conditions with the same catalyst at 800 °C. A 100 h continuous operation of this process was carried out and the result indicates the feasibility for practical applications.

L24 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

TI Direct conversion of 2-methylglutaronitrile to 3-picoline and cyclic amines

AU Heveling, Josef

SO Chemical Industries (Dekker) (1996), 68(Catalysis of Organic Reactions), 265-276

CODEN: CHEIDI; ISSN: 0737-8025

AB 3-Picoline was prepared in one step from 2-methylglutaronitrile (MGN) over a

fixed-bed Pd/ Al_2O_3 -catalyst. In this case, the sequence of a hydrogenation reaction, a cyclization reaction and a dehydrogenation reaction took place in one reactor over the same catalyst. The window for the reaction conditions, which allowed this reaction to proceed, was very narrow; namely a reactor temperature of 280-290°C and a pressure (H_2) of approx. 500 kPa. This reaction was accompanied by a rapid catalyst deactivation, and afterwards a viscous dark oil was extracted from the catalyst bed. This oil had a mol. mass of 500-3000 and was mainly aliphatic in nature. It was probably formed via the polymerization of imine intermediates

and was the main cause of catalyst deactivation. Over the same catalyst at 180°C/5 MPa a water-clear, oily substance was formed without obvious catalyst deactivation. It was identified as 1,1'-(2-methyl-1,5-pentanediy)bis[3-methylpiperidine]. This reaction was extended to glutaronitrile and adipodinitrile as substrates. At a somewhat lower temperature and with the addition of approx. two moles of 3-methylpiperidine per mol of MGN, a mixture of 2-methyl- and 4-methyl-5-(3-methylpiperidino)pentanenitrile became the main product. This mixture (after saturation of the nitrile group) was active as a migration inhibited polyurethane catalyst.

L29 ANSWER 1 OF 15 USPATFULL on STN

TI Catalytic reactor with integral evaporator

IN Karlsson, Arne, Oslo, NORWAY

Dahl, Ivar M., Oslo, NORWAY

Engedahl, Jonny, Oslo, NORWAY

Krawczyk, Mark A., Chicago, IL, UNITED STATES

Alexanian, Ara J., Des Plaines, IL, UNITED STATES

PI US 2003175173 A1 20030918

AI US 2002-95934 A1 20020312 (10)

AB A reactor for evaporating liquid feed and reacting said feed in the presence of catalyst to make product comprises a housing having at least

- one inlet and at least one outlet and encasing an evaporation zone and a reaction zone, an injector passing through the inlet and having an orifice in the evaporation zone for introducing a liquid feed, an insert containing packing for vaporizing the liquid feed where the packing is in the evaporation zone, a receptacle for retaining catalyst in the reaction zone and at least one heater associated with at least a portion of the reactor, wherein the injector orifice and the packing define a gap between the orifice and the packing sufficiently small to interfere with the formation of a drop at the orifice.

L29 ANSWER 2 OF 15 USPATFULL on STN

TI Process vessel with integral evaporator
IN Karlsson, Arne, Oslo, NORWAY
Dahl, Ivar M., Oslo, NORWAY
Engedahl, Jonny, Oslo, NORWAY
Krawczyk, Mark A., Chicago, IL, UNITED STATES
Alexanian, Ara J., Des Plaines, IL, UNITED STATES

PI US 2003173205 A1 20030918

AI US 2002-95879 A1 20020312 (10)

AB A process vessel containing both an evaporation zone for evaporating a liquid feed and a treatment zone for treating the resulting vapor comprises an injector having an orifice, the orifice being in the evaporation zone, at least one evaporation surface for evaporating feed and generating vapor, the evaporation surface being located in the evaporation zone, wherein the injector orifice and the evaporation surface are positioned to prevent the formation of a drop at the orifice, a treatment zone for treating the vapor and at least one heater associated with at least a portion of the process vessel.

L29 ANSWER 3 OF 15 USPATFULL on STN

TI Integrated hydrogen peroxide production and organic chemical oxidation
IN Zhou, Bing, Cranbury, NJ, United States
Rueter, Michael, Plymouth Meeting, PA, United States
PI US 6500969 B1 20021231
PA Hydrocarbon Technologies, Inc., Lawrenceville, NJ, United States (U.S. corporation)

AI US 2001-14068 20011211 (10)

AB A process for producing oxidized organic chemical products from various organic chemical feedstocks utilizing as oxidant hydrogen peroxide (H₂O₂) produced by noble metal nanocatalysis with high selectivity at low hydrogen concentration. The organic chemical oxidation process step can optionally be carried out in situ concurrent with the production of hydrogen peroxide or in a two stage process. In the two stage process, the hydrogen peroxide intermediate is directly produced by noble metal nanocatalysis from hydrogen and oxygen feeds plus a suitable solvent in a first catalytic reaction step. An organic chemical feedstock and the hydrogen peroxide intermediate and solvent solution are fed into a second catalytic reactor to produce an oxidized organic chemical product.

L29 ANSWER 4 OF 15 USPATFULL on STN

TI Parallel flow reactor having improved thermal control
IN Bergh, H. Sam, San Francisco, CA, UNITED STATES
Guan, Shenheng, Palo Alto, CA, UNITED STATES
Engstrom, James R., Ithaca, CA, UNITED STATES
Hardt, Steffen, Mainz, CA, UNITED STATES
Lohf, Astrid, Karlsruhe, GERMANY, FEDERAL REPUBLIC OF
Michel, Frank, Bad Mergentheim, GERMANY, FEDERAL REPUBLIC OF

PI US 2002170976 A1 20021121

AI US 2002-94257 A1 20020307 (10)

AB Parallel flow chemical processing systems, such as parallel flow chemical reaction systems are disclosed. These systems are adapted to simultaneously and independently vary temperature between separate flow channels, preferably by employing separate, individual heating elements in thermal communication with each of four or more parallel flow reactors. The flow reactors are preferably isolated from each other using a thermal isolation system comprising fluid-based heat exchange. In preferred embodiments, the axial heat flux can be fixedly or controllably varied.

L29 ANSWER 5 OF 15 USPATFULL on STN

TI Methods for analysis of heterogeneous catalysts in a multi-variable screening reactor
IN Hagemeyer, Alfred, Sunnyvale, CA, UNITED STATES
Volpe, Anthony F., JR., Santa Clara, CA, UNITED STATES
Lugmair, Claus, San Jose, CA, UNITED STATES
Lowe, David M., Mt. View, CA, UNITED STATES
Liu, Yumin, San Jose, CA, UNITED STATES

Bergh, H. Sam, San Francisco, CA, UNITED STATES
Guan, Shenheng, Palo Alto, CA, UNITED STATES
Pinkas, Daniel M., Alameda, CA, UNITED STATES
Self, Kyle W., San Jose, CA, UNITED STATES
Engstrom, James R., Ithaca, NY, UNITED STATES
Lefort, Laurent, Ashland, OR, UNITED STATES

PI US 2002042140 A1 20020411

AI US 2001-901858 A1 20010709 (9)

AB Protocols for designing and implementing sets of simultaneous experiments, in a parallel, multi-variable process optimization reactor, are disclosed. The multi-variable process optimization reactor is preferably a parallel flow reactor having the operational capability to simultaneously vary reaction conditions between reaction vessels--either modularly or independently. The simultaneously varied reaction conditions preferably include at least two of the following, in various combinations and permutations: space velocity, contact time, temperature, pressure and feed composition. Compositional variations in the catalysts residing in each of the reaction vessels can also be investigated in the set of simultaneous experiments implemented in the parallel reactor. Sufficient data is obtained from a single set of simultaneous experiments to generate a master curve.

L29 ANSWER 6 OF 15 USPATFULL on STN

TI Methods and equipments of using dual functional catalyst of packing type
IN Gao, Buliang, Shandong Province, China
Zhang, Jinyong, Shandong Province, China
Wang, Jinshan, Shandong Province, China
Hao, Xingren, Shandong Province, China
Yu, Zaiqun, Shandong Province, China
Wang, Wei, Shandong Province, China

PI US 6291719 B1 20010918

PA China Petro-Chemical Corporation, Beijing, China (non-U.S. corporation)
Qilu Petro-Chemical Corporation Sinopec, Zibo, China (non-U.S. corporation)

AI US 2000-650094 20000829 (9)

AB The present invention relates to a method of catalyzing etherification, esterification, hydration, ether cleavage, isomerization alkylation, or other reactions which are catalyzable with an acid or molecular sieve catalyst. Said reactions are conducted using a novel, dual functional catalyst prepared with active components and a small amount of binder, wherein said dual functional catalyst comprises cylindrical pellets which are molded such that a cross-section of each pellet has a window lattice shape with external teeth, or a star shape with inner spokes.

L29 ANSWER 7 OF 15 USPATFULL on STN

TI Dual functional catalyst of packing type and the catalytic distillation equipment

IN Gao, Buliang, Shandong Province, China
Zhang, Jinyong, Shandong Province, China
Wang, Jinshan, Shandong Province, China
Hao, Xingren, Shandong Province, China
Yu, Zaiqun, Shandong Province, China
Wang, Wei, Shandong Province, China

PI US 6117812 20000912

PA China Petro-Chemical Corporation, Beijing, China (non-U.S. corporation)
Qilu Petro-Chemical Corporation Sinopec, Zibo, China (non-U.S. corporation)

AI US 1998-166931 19981006 (9)

AB The present invention relates to a dual functional catalyst having both the catalytic reaction function and fractionation function and a catalytic distillation equipment for packing the catalyst therein. Said catalyst has a special shape and can be packed at random into the reaction section of said equipment. So, there exist adequate free spaces inside pellet and between pellets, enabling the vapor and liquid streams to pass through the catalyst beds directly and countercurrently, and contact with the dual functional catalyst directly. The reaction between the reactants and fractionation of products can be carried out simultaneously. Thus a high reaction efficiency is achieved. No special inner part is needed in the reaction section to pack the catalysts, so the structure of the equipment is simple and easy to operate, and the investment and cost of operation are low.

L29 ANSWER 8 OF 15 USPATFULL on STN

TI Process for preparing iodinated aromatic compounds
IN Rule, Mark, Kingsport, TN, United States
Lane, Donald W., Kingsport, TN, United States
Larkins, Thomas H., Kingsport, TN, United States

- Tustin, Gerald C., Kingsport, TN, United States
PI US 4792641 19881220
PA Eastman Kodak Company, Rochester, NY, United States (U.S. corporation)
- AI US 1987-29899 19870325 (7)
AB The invention relates to a process for isomerizing and transiodinating iodoaromatic compounds over a non-acid catalyst.

L29 ANSWER 9 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN TIEN ORGANIC CHEMICAL OXIDATION DURING HYDROGEN PEROXIDE PRODUCTION
TIFR OXYDATION CHIMIQUE ORGANIQUE PENDANT LA PRODUCTION DE PEROXYDE D'HYDROGENE

IN ZHOU, Bing, 2 Falcon Ct., Cranbury, NJ 08512, US [US, CA];
RUETER, Michael, 350 Maiden Lane, Plymouth Meeting, PA 19462, US [US, —]

PI WO 2004009570 A1 20040129
PA HYDROCARBON TECHNOLOGIES, INC., 1501 New York Avenue, Lawrenceville, NJ 08648, US [US, US];
ZHOU, Bing, 2 Falcon Ct., Cranbury, NJ 08512, US [US, CA];
RUETER, Michael, 350 Maiden Lane, Plymouth Meeting, PA 19462, US [US, —]

AI WO 2002-US32623 A 20021011

ABEN A process for producing oxidized organic chemical products from various

organic chemical feedstocks utilizing as oxidant hydrogen peroxide (H2O2) produced by noble metal nanocatalysis with high selectivity at low hydrogen concentration. The organic chemical oxidation process step can optionally be carried out in situ concurrent with the production of hydrogen peroxide or in a two stage process. In the two stage process, the hydrogen peroxide intermediate is directly produced by noble metal nanocatalysis from hydrogen and oxygen feeds plus a suitable solvent in a first catalytic reaction step. An organic chemical feedstock and the hydrogen peroxide intermediate and solvent solution are fed into a second catalytic reactor to produce an oxidized organic chemical product.

ABFR L'invention concerne un procede de production de produits chimiques organiques oxydes a partir de diverses charges chimiques organiques au moyen de peroxyde d'hydrogene oxydant (H2O2) produit au moyen d'une nanocatalyse de metal noble avec une selectivite elevee a de faible teneur en hydrogene. L'etape du procede d'oxydation chimique organique peut etre effectuee eventuellement <i>in situ</i> en meme temps que la production de peroxyde d'hydrogene ou dans un procede en deux etapes dans lequel l'intermediaire de peroxyde d'hydrogene est produit directement au moyen de la nanocatalyse de metal noble a partir de charges d'hydrogene et d'oxygene, ainsi que d'un solvant approprie dans la premiere etape de reaction catalytique. Une charge chimique organique, l'intermediaire de peroxyde d'hydrogene et la solution de solvant sont alimentes dans un second reacteur catalytique, de maniere a produire un produit chimique organique oxyde.

US only;
DAHL, Ivar, M., SINTEF, 124 Blindern, N-0314, N- Oslo, NO [NO, NO],

for
US only;
ENGEDAHL, Jonny, SINTEF, 124 Blindern, N-0314, N- Oslo, NO [NO, NO], for

US only;
KRAWCZYK, Mark, A., UOP LLC, 25 East Algonquin Road, DES PLAINES, IL 60017-5017, US [US, US], for US only;
ALEXANIAN, Ara, J., UOP LLC, 25 EAST ALGONQUIN ROAD, DES PLAINES, IL

60017-5017, US [US, US], for US only

AI WO 2003-US8228 A 20030310

ABEN A process for evaporating a feed liquid and a process vessel (10) containing both an evaporation zone (18) for evaporating a liquid feed and a treatment zone (26) for treating the resulting vapor uses an evaporation surface (82) to prevent the formation of liquid droplets. The apparatus comprises an injector (48) having an orifice (66), the orifice (66) being in the evaporation zone (18), at least one evaporation surface (82) for evaporating feed and generating vapor, the evaporation surface (82) being located in the evaporation zone (18), wherein the injector orifice and the evaporation surface (82) are positioned to prevent the formation of a drop at the orifice (66), a treatment zone (26) for treating the vapor and at least one heater (20) associated with at least a portion of the process vessel.

ABFR L'invention concerne un procede relatif a l'evaporation de charge de liquide et un recipient de mise en oeuvre (10), qui comprend une zone d'evaporation (18) pour l'evaporation d'une charge de liquide, et une zone de traitement (26) pour le traitement de la vapeur resultante. On utilise une surface d'evaporation (82) pour eviter la formation de gouttelettes de liquide. Le dispositif presente aussi un injecteur (48) comprenant un orifice (66), lequel (66) est situe dans la zone d'evaporation (18), et au moins une surface d'evaporation (82) pour l'evaporation de la charge et la production de vapeur. La surface d'evaporation (82) se trouve dans la zone d'evaporation (18). L'orifice de l'injecteur et la surface d'evaporation (82) ont un positionnement permettant d'eviter la formation d'une gouttelette a l'orifice (66). Il existe enfin une zone de traitement (26) pour le traitement de la vapeur, et au moins une unite chauffante (20) associee au moins a une partie du recipient de mise en oeuvre.

L29 ANSWER 11 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN TIEN PROCESS FOR EVAPORATION IN AN ARRAY AND AN ARRAY OF PROCESS VESSELS WITH INTEGRAL EVAPORATOR

TIFR PROCEDE D'EVAPORATION DANS UN RESEAU ET RESEAU DE CUVES DE TRAITEMENT A EVAPORATEUR INTEGRE

IN KARLSSON, Arne, SINTEF, 124 Blindern, N-0314 Oslo, NO [SE, NO];
DAHL, Ivar, M., SINTEF, 124 Blindern, N-0314 Oslo, NO [NO, NO];
ENGEDAHL, Jonny, SINTEF, 124 Blindern, N-0314 Oslo, NO [NO, NO];
KRAWCZYK, Mark, A., UOP LLC, 25 East Algonquin Road, Des Plaines, IL

60017-5017, US [US, US];

ALEXANIAN, Ara, J., UOP LLC, 25 East Algonquin Road, Des Plaines, IL

60017-5017, US [US, US]

PI WO 2003078051 A2 20030925

PA UOP LLC, 25 East Algonquin Road, Des Plaines, IL 60017-5017, US [US, US], for all designates States except US;

KARLSSON, Arne, SINTEF, 124 Blindern, N-0314 Oslo, NO [SE, NO], for US only;

DAHL, Ivar, M., SINTEF, 124 Blindern, N-0314 Oslo, NO [NO, NO], for US only;

ENGEDAHL, Jonny, SINTEF, 124 Blindern, N-0314 Oslo, NO [NO, NO], for US only;

KRAWCZYK, Mark, A., UOP LLC, 25 East Algonquin Road, Des Plaines, IL 60017-5017, US [US, US], for US only;
ALEXANIAN, Ara, J., UOP LLC, 25 East Algonquin Road, Des Plaines, IL 60017-5017, US [US, US], for US only

AI WO 2003-US7061 A 20030310

ABEN A process for evaporating a feed liquid and a process vessel containing both an evaporation zone for evaporating a liquid feed and a treatment zone for treating the resulting vapor uses an evaporation surface to

L29 ANSWER 10 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN TIEN PROCESS FOR EVAPORATION AND PROCESS VESSEL WITH INTEGRAL EVAPORATOR

TIFR PROCEDE D'EVAPORATION, ET RECIPIENT DE MISE EN OEUVRE A EVAPORATEUR INTEGRE

IN KARLSSON, Arne, SINTEF, 124 Blindern, N-0314, N- Oslo, NO [SE, NO];
DAHL, Ivar, M., SINTEF, 124 Blindern, N-0314, N- Oslo, NO [NO, NO];
ENGEDAHL, Jonny, SINTEF, 124 Blindern, N-0314, N- Oslo, NO [NO, NO];

KRAWCZYK, Mark, A., UOP LLC, 25 East Algonquin Road, DES PLAINES, IL

60017-5017, US [US, US];

ALEXANIAN, Ara, J., UOP LLC, 25 EAST ALGONQUIN ROAD, DES PLAINES, IL

60017-5017, US [US, US]

PI WO 2003078053 A1 20030925

PA UOP LLC, 25 EAST ALGONQUIN ROAD, DES PLAINES, IL 60017-5017, US [US,

US], for all designates States except US;

KARLSSON, Arne, SINTEF, 124 Blindern, N-0314, N- Oslo, NO [SE, NO], for

prevent the formation of liquid droplets. The apparatus may comprise an injector having an orifice, the orifice being in the evaporation zone, at least one evaporation surface for evaporating feed and generating vapor, the evaporation surface being located in the evaporation zone, wherein the injector orifice and the evaporation surface are positioned to prevent the formation of a drop at the orifice, a treatment zone for treating the vapor and at least one heater associated with at least a portion of the process vessel.

ABFR L'invention concerne un procede d'evaporation d'une alimentation liquide, et une cuve de traitement contenant une zone d'evaporation permettant d'evaporer une alimentation liquide et une zone de traitement permettant de traiter la vapeur obtenue, qui met en oeuvre une surface d'evaporation destinee a empecher la formation de gouttelettes liquides. Cet appareil peut comprendre: un injecteur presentant un orifice situe dans la zone d'evaporation; au moins une surface d'evaporation situee dans ladite zone d'evaporation qui permet d'evaporer l'alimentation et de produire de la vapeur, l'orifice de l'injecteur et la surface d'evaporation etant positionnees de maniere a empecher la formation d'une goutte au niveau dudit orifice; une zone de traitement qui permet de traiter la vapeur; et au moins un element chauffant associe a au moins une partie de ladite cuve de traitement.

L29 ANSWER 12 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN TIEN METHODS FOR ANALYSIS OF HETEROGENEOUS CATALYSTS IN A MULTI-VARIABLE

SCREENING REACTOR

TIFR ANALYSE DE CATALYSEURS HETEROGENES DANS UN REACTEUR DE CRIBLAGE MULTI-CRITERE

IN HAGEMEYER, Alfred;
VOLPE, Anthony, F., Jr.;
LEFORT, Laurent;
LUGMAIR, Claus;
LOWE, David, M.;
LIU, Yumin;
BERGH, H., Sam;
GUAN, Shenheng;
PINKAS, Daniel, M.;
ENGSTROM, James, R.;
SELF, Kyle, W.

PI WO 2002004112 A2 20020117

PA SYMYX TECHNOLOGIES, INC.

AI WO 2001-US21718 A 20010709

ABEN Protocols for designing and implementing sets of simultaneous experiments, in a parallel, multi-variable process optimization reactor, are disclosed. The multi-variable process optimization reactor is preferably a parallel flow reactor having the operational capability to simultaneously vary reaction conditions between reaction vessels - either modularly or independently. The simultaneously varied reaction conditions preferably include at least two of the following, in various combinations and permutations: space velocity, contact time, temperature, pressure and feed composition. Compositional variations in the catalysts residing in each of the reaction vessels can also be investigated in the set of simultaneous experiments implemented in the parallel reactor. Sufficient data is obtained from a single set of simultaneous experiments to generate a master curve.

ABFR La presente invention concerne des protocoles de conception et de mise en oeuvre de jeux d'experiences simultanees dans un reacteur d'optimisation de processus multicriteres paralleles. Ce reacteur d'optimisation de processus multicriteres paralleles est de preference un reacteur a flux paralleles fonctionnellement capable de faire varier simultanement des conditions d'une cuve de reaction a l'autre, soit par modules, soit independamment les unes des autres. Pour faire varier les conditions de reaction simultanement, on peut agir selon differentes configurations d'association et de permutation sur les parametres que sont la vitesse volumique, les temps de contact, la temperature, la pression, et la composition du produit de depart. Les variations de composition des catalyseurs des differentes cuves de reaction peuvent egalement faire l'objet de recherche dans le jeu d'experiences simultanees mis en oeuvre dans le reacteur en parallele. Un meme jeu d'experiences simultanees donne suffisamment de donnees pour l'etablissement d'une courbe de reference.

DELORME, Luc, Avenue des Petits Champs 10, B-1410 Waterloo, BE;
GROOTJANS, Jacques-Francois, Neeryresteenweg 39, B-3061 Leefdaal, BE;
VANHAEREN, Xavier, Vieux Chemin de l'Helpe 63, B-1332 Genval, BE;
VERMEIREN, Walter, Winningstraat 4, B-3530 Houthalen, BE
PI EP 1036138 B1 20030528
PA ATOFINA Research, Zone Industrielle C, 7181 Seneffe (Feluy), BE
AI EP 1998-958742 19981207

L29 ANSWER 14 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN

TIEN PRODUCTION OF OLEFINS.

IN DATH, Jean-Pierre, Rue d'Ath 53, B-7970 Beloeil, BE;
DELORME, Luc, Avenue des Petits Champs 10, B-1410 Waterloo, BE;
GROOTJANS, Jacques-Francois, Neeryresteenweg 39, B-3061 Leefdaal, BE;
VANHAEREN, Xavier, Vieux Chemin de l'Helpe 63, B-1332 Genval, BE;
VERMEIREN, Walter, Winningstraat 4, b-3530 Houthalen, BE
PI EP 1036135 B1 20020911
PA ATOFINA Research, Zone Industrielle C, 7181 Seneffe (Feluy), BE
AI EP 1998-958125 19981207

L29 ANSWER 15 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN

TIEN PRODUCTION OF OLEFINS.

IN DATH, Jean-Pierre, Rue d'Ath 53, B-7970 Beloeil, BE;
DELORME, Luc, Avenue des Petits Champs 10, B-1410 Waterloo, BE;
GROOTJANS, Jacques-Francois, Neeryresteenweg 39, B-3061 Leefdaal, BE;
VANHAEREN, Xavier, Vieux Chemin de l'Helpe 63, B-1332 Genval, BE;
VERMEIREN, Walter, Winningstraat 4, B-3530 Houthalen, BE
PI EP 1036133 B1 20030702
PA ATOFINA Research, Zone Industrielle C, 7181 Seneffe (Feluy), BE
AI EP 1998-958122 19981207

L29 ANSWER 13 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN

TIEN PRODUCTION OF OLEFINS.

IN DATH, Jean-Pierre, Rue d'Ath 53, B-7970 Beloeil, BE;

ANSWER SUMMARY

L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231; 2003:761541 CAPLUS

L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231

L6 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Scalability of Microwave-Assisted Organic Synthesis. From Single-Mode to Multimode Parallel Batch Reactors

L6 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Microwave assisted reactions with arylboronic acids

L6 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions and stabilization of phenylalanine ammonia lyase-containing *Rhodotorula glutinis* cells during bioconversion of trans-cinnamic acid to L-phenylalanine

L6 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Parallel catalyst screening instrumentation

L6 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Removal of ammonia and phenol by using hydrophobic catalyst

L6 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; 6,6-Dimethylhept-1-en-4-yn-3-ol: a useful model for investigation of the effect of trifluoroacetic acid on the stereoselectivity of allylic rearrangement

L6 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Investigation of conditions in porphyrin-forming reactions using an automated chemistry workstation

L6 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Factors which affect the catalytic activity of iron(III) meso tetrakis(2,6-dichlorophenyl)porphyrin chloride in homogeneous system

L6 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; The diffusion model of solid-state catalytic hydrogen isotope exchange. Isoradiochemical purity dependencies of the exchange level on temperature for thymine

L6 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic addition of formaldehyde to unsaturated oleochemicals

L6 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Substitution catalytic hydrogenation of C2 chloro derivatives

L6 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Ethylene from natural gas by direct catalytic oxidation

L6 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Methane steam reforming: II. Diffusional limitations and reactor simulation

L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231; 2003:761541 CAPLUS

L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231; 2003:761541 CAPLUS

L6 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Removal of ammonia and phenol by using hydrophobic catalyst

L6 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Parallel catalyst screening instrumentation

L10 ANSWER 1 OF 84 CAPLUS COPYRIGHT 2004 ACS on STN; Reactivity of triglycerides and fatty acids of rapeseed oil in supercritical alcohols

L12 ANSWER 1 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 11 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

L12 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
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 L12 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
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 L12 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
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 L12 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
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 L12 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
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 L12 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
 L12 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Operando resonance Raman spectroscopic characterization of the oxidation state of palladium in Pd/ γ -Al₂O₃ catalysts during the combustion of methane
 L12 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic Raman spectroscopy: the operando approach
 L12 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; A Raman Spectroscopy Study of Alumina-Supported Vanadium Oxide Catalyst during Propane Oxidative Dehydrogenation with Online Activity Measurement
 L12 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Parallel catalyst screening instrumentation
 L14 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

L14 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L14 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN
 L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231
 L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions for biocatalytic resolution of (R,S)-4-hydroxy-3-methyl-2-(2-propenyl)-cyclopent-2-enone by resting cells of *Acinetobacter* sp. YQ231
 L6 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Scalability of Microwave-Assisted Organic Synthesis. From Single-Mode to Multimode Parallel Batch Reactors
 L6 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Microwave assisted reactions with arylboronic acids
 L6 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Optimization of reaction conditions and stabilization of phenylalanine ammonia lyase-containing *Rhodotorula glutinis* cells during bioconversion of trans-cinnamic acid to L-phenylalanine
 L6 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Parallel catalyst screening instrumentation
 L6 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Removal of ammonia and phenol by using hydrophobic catalyst
 L6 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; 6,6-Dimethylhept-1-en-4-yn-3-ol: a useful model for investigation of the effect of trifluoroacetic acid on the stereoselectivity of allylic rearrangement
 L6 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Investigation of conditions in porphyrin-forming reactions using an automated chemistry workstation
 L6 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Factors which affect the catalytic activity of iron(III) meso tetrakis(2,6-dichlorophenyl)porphyrin chloride in homogeneous system
 L6 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; The diffusion model of solid-state catalytic hydrogen isotope exchange. Isoradiochemical purity dependencies of the exchange level on temperature for thymine
 L6 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic addition of formaldehyde to unsaturated oleochemicals
 L6 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Substitution catalytic hydrogenation of C2 chloro derivatives
 L6 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Ethylene from natural gas by direct catalytic oxidation
 L6 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2004 ACS on STN; Methane steam reforming: II. Diffusional limitations and reactor simulation
 L12 ANSWER 1 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Reactivity of triglycerides and fatty acids of rapeseed oil in supercritical alcohols
 L12 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Palladium-Catalyzed Carbonylative Annulation of Internal Alkynes: Synthesis of 3,4-Disubstituted Coumarins
 L12 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Comparing catalytic distillation to separate reaction and distillation for the production of diacetone alcohol
 L12 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Iron-containing silicalites for phenol catalytic wet peroxidation
 L12 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; A highly active and reusable heterogeneous catalyst for the Suzuki reaction: synthesis of biaryls and polyaryls
 L12 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Operando resonance Raman spectroscopic characterization of the oxidation state of palladium in Pd/ γ -Al₂O₃ catalysts during the combustion of methane
 L12 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic Raman spectroscopy: the operando approach
 L12 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Selective Oxidation of Propylene to Propylene Oxide by Molecular Oxygen over Ti-Al-HMS Catalysts
 L12 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Production of diethyl carbonate from ethanol and carbon monoxide over a heterogeneous catalytic flow reactor

L12 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Synthesis of 2 - methyl - 3 - (3,4 - methylenedioxyphenyl) acraldehyde by $\text{KF}/\text{Al}_2\text{O}_3$ catalyst

L12 ANSWER 11 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Enantioselective Total Synthesis of (-)-Strychnine Using the Catalytic Asymmetric Michael Reaction and Tandem Cyclization

L12 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; A Raman Spectroscopy Study of Alumina-Supported Vanadium Oxide Catalyst during Propane Oxidative Dehydrogenation with Online Activity Measurement

L12 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Simultaneous determination of reaction kinetics and oxygen activity in single-phase oxidic catalysts and their mixture during partial oxidations

L12 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Molecular structures of supported metal oxide catalysts under different environments

L12 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Evaluation of catalytic cracking catalyst for reducing sulfur content in gasoline

L12 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic Reduction of NO and N_2O to N_2 in the Presence of O_2 , C_3H_6 , SO_2 , and H_2O

L12 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Microfabricated cross-flow chemical reactor for catalyst testing

L12 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; The methane reforming with carbon dioxide on Ni-catalyst activated by a DC-pulsed corona discharge

L12 ANSWER 19 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Automated Library Generation Using Sequential Microwave-Assisted Chemistry. Application toward the Biginelli Multicomponent Condensation

L12 ANSWER 20 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Structural change and catalytic activity of horseradish peroxidase in oxidative polymerization of phenol

L12 ANSWER 21 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Study on hydroetherification of FCC light gasoline using Pd/ion exchanger resin catalyst

L12 ANSWER 22 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; In situ studies of atomic, nano- and macroscale order during $\text{VOHPO}_4 \cdot 0.5\text{H}_2\text{O}$ transformation to $(\text{VO})_2\text{P}_2\text{O}_7$

L12 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Parallel catalyst screening instrumentation

L12 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; An experimental and theoretical investigation of a catalytic membrane reactor for the oxidative dehydrogenation of methanol

L12 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Unraveling catalytic kinetics via detailed mechanistic modeling and computational chemistry.

L12 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Manufacture of carbonylation products, aldehydes and/or alcohols, esters from the alcohols, ester plasticizers, and thermoplastic resins

L12 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Shape-selective synthesis of 4,4'-dimethylbiphenyl. 1. Methylation of 4-methylbiphenyl over modified zeolite catalysts

L12 ANSWER 28 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Activity, Selectivity, and Sulfur Resistance of $\text{Pt}/\text{WO}_x\text{-ZrO}_2$ and Pt/Beta Catalysts for the Simultaneous Hydroisomerization of n-Heptane and Hydrogenation of Benzene

L12 ANSWER 29 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Hydrodechlorination and hydrodearomatization of monoaromatic chlorophenols into cyclohexanol on Ru/C catalysts applied to water depollution. Influence of the basic solvent and kinetics of the reactions

L12 ANSWER 30 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Experimental study on selectivities of Fischer-Tropsch synthesis over a Fe-Cu-K catalyst

L12 ANSWER 31 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Effect of cobalt chloride on the regioselectivity of reaction of olefins with carbon monoxide and alcohols, catalyzed with $\text{PdCl}_2(\text{Ph}_3\text{P})_2$

L12 ANSWER 32 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Effect of the addition of chromium- and manganese oxides on structural and catalytic properties of copper/zirconia catalysts for the synthesis of methanol from carbon dioxide

L12 ANSWER 33 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Oxidative coupling of methane over $\text{SrF}_2/\text{Y}_2\text{O}_3$ catalyst

L12 ANSWER 34 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Analytical derivatizations of volatile and hydrophilic carbonyls from aqueous matrix onto a solid phase of a polystyrene-divinylbenzene macroreticular resin

L12 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Partial oxidation of methane to synthesis gas using LnCoO_3 perovskites as catalyst precursors

L12 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Reaction engineering studies in a polytropic fixed-bed reactor over a highly active and selective catalyst for oxidative methane coupling

L12 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic behavior of multiphasic oxide catalysts containing lanthanides (La , Ce , Pr , Sm , Tb) in the selective oxidation of

isobutene to methacrolein

L12 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Promoter effect of cesium on C-C bond formation during alcohol synthesis from CO/H₂ over Cu/ZnO/Cr₂O₃ catalysts

L12 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Unique fractionation of biomass to polyols provides inexpensive feedstock for liquid fuels process

L12 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Isobutane/2-butene alkylation over faujasite type zeolites in a slurry reactor. Effect of operating conditions and catalyst regeneration

L12 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Energy efficient methane-to-syngas conversion with low H₂/CO ratio by simultaneous catalytic reactions of methane with carbon dioxide and oxygen

L12 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Gas-phase one-step preparation of 1, 4-butanediol and γ -butyrolactone

L12 ANSWER 43 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; A simplified kinetic model for Illinois No.6 coal liquefaction

L12 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Mechanism and Dynamics in the H₃[PW₁₂O₄₀]-Catalyzed Selective Epoxidation of Terminal Olefins by H₂O₂. Formation, Reactivity, and Stability of {PO₄[WO(O₂)₂]₄}³⁻

L12 ANSWER 45 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Morphology changes and deactivation of alkali-promoted Ni/SiO₂ catalysts during carbon monoxide hydrogenation

L12 ANSWER 46 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Hydrogenation of carbon dioxide over copper, silver and gold/zirconia catalysts: comparative study of catalyst properties and reaction pathways

L12 ANSWER 47 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Selective oxidation of methane with air over silica catalysts

L12 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Kinetics and reaction network in propane ammoxidation to acrylonitrile on vanadium-antimony-aluminum based mixed oxides

L12 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Ethylene from natural gas by direct catalytic oxidation

L12 ANSWER 50 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; The production of hydroxylamine by hydration of nitrate on suspended palladium/carbon catalyst: kinetics and mass transfer

L12 ANSWER 51 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Selective thermal cracking of heavy oil (Part 5). Selective thermal cracking of Kuwait atmospheric residue by using carbon monoxide shift reaction

L12 ANSWER 52 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; 1,8-Naphthalenecarbolactone and acenaphthenone in liquid-phase oxidation of acenaphthene to naphthalic anhydride

L12 ANSWER 53 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Rhodium on chromia-alumina catalysts for toluene steam-dealkylation: characteristics and catalytic behavior

L12 ANSWER 54 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Chloroform deuteration

L12 ANSWER 55 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Hydrogenation of furfural on copper-zirconium Raney-type catalysts under hydrogen pressure

L12 ANSWER 56 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Simultaneous manufacture of methacrylonitrile and butadiene by catalytic vapor-phase oxidation of mixed butenes

L12 ANSWER 57 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Vapor-phase catalytic re-esterification of ethyl acetate with methanol

L12 ANSWER 58 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Relation between catalytic and electric properties of germanium and its isoelectronic analogs

L12 ANSWER 59 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Autoxidation of quinoline 1-oxide

L12 ANSWER 60 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Metalation of N,N-dimethylaniline

L12 ANSWER 61 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic synthesis of dimethylcyclopentadienes

L12 ANSWER 62 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Tritium labeling of natural products

L12 ANSWER 63 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Synthesis of α - and γ -picoline by a vapor-phase catalytic reaction. I. Reaction products and the reaction conditions

L12 ANSWER 64 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Naphtha hydroforming by irradiation

L12 ANSWER 65 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Kinetic equations for heptane reactions under catalytic reforming conditions

L12 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Organosilicon compounds. XXVIII. Direct synthesis of ethylchlorosilanes

L12 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Reactor and regenerator for fluid catalytic cracking

L12 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN; Aluminum halide-olefinic ketone complexes as catalyst for hydrocarbon reactions

L14 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Ethylene oligomerization with Ni(MeCN)₆(BF₄)₂ in homogeneous phase, immobilized in ionic liquids or heterogenized in zeolite

L14 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Fischer-Tropsch synthesis: induction

and steady-state activity of high-alpha potassium promoted iron catalysts

L14 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Dimerization of 1-butene catalyzed by zirconium complexes

L14 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; A novel cross-aldol condensation for preparation of hydroxypivaldehyde using simple phase-transfer catalysts

L14 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Process for the preparation of olefin oxides

L14 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Oxidative coupling of methane as a method for natural gas chemical utilization

L14 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Stability test of MgO/BaCO₃ catalyst for oxidative coupling of methane in fixed-bed reactor

L14 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Selectivity control by oxygen pressure in methane oxidation over phosphate catalysts

L14 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Selectivity control by oxygen pressure in methane oxidation over phosphate catalysts

L14 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Base- and acid-catalysed cyclization of diketones over ZSM-5

L14 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Tin analogs of the vinylogous Reformatsky reaction. Regio- and stereochemical considerations

L14 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Reaction of chlorobenzene, carbon monoxide and benzene under high pressure

L14 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Activation of catalysts by γ -rays for the manufacture of gas

L14 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Long chain vinyl ethers and esters, their polymers and copolymers. II. Preparation, purification, and Characterization of some long chain vinyl esters

L14 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Aromatic hydrocarbons from diarylalkanes

L14 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN; Methylchlorosilanes

L16 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane

L16 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; n-Hexane oxyfunctionalization by hydrogen peroxide over titanium silicalite containing catalytic membranes

L16 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; Catalytic performance of an ultrafine Cu/ZnO/Al₂O₃ catalyst prepared by gel-oxalate coprecipitation

L16 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; Application of Cu-Pd composite membranes in dehydrogenation of methanol to methyl formate

L16 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; Synthesis of dimethyl ether and alternative fuels in the liquid phase from coal-derived synthesis gas: Task 3.2: Screen novel catalyst systems; Task 3.3: Evaluation of the preferred catalyst system

L16 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN; Poly- or copolymerization of ethylene by gas phase method by using a fluidized bed reactor

L18 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN; Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane

L18 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN; Application of Cu-Pd composite membranes in dehydrogenation of methanol to methyl formate

L18 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN; A comparison of the fixed-bed, liquid-phase ("slurry") and fluidized-bed techniques in the Fischer-Tropsch synthesis

L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN; A comparison of the fixed-bed, liquid-phase ("slurry") and fluidized-bed techniques in the Fischer-Tropsch synthesis

L24 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN; Continuous oxygen ion transfer medium as a catalyst for high selective oxidative dehydrogenation of ethane

L24 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN; Direct conversion of 2-methylglutaronitrile to 3-picoline and cyclic amines

L29 ANSWER 1 OF 15 USPATFULL on STN; Catalytic reactor with integral evaporator

L29 ANSWER 2 OF 15 USPATFULL on STN; Process vessel with integral evaporator

L29 ANSWER 3 OF 15 USPATFULL on STN; Integrated hydrogen peroxide production and organic chemical oxidation

L29 ANSWER 4 OF 15 USPATFULL on STN; Parallel flow reactor having improved thermal control

L29 ANSWER 5 OF 15 USPATFULL on STN; Methods for analysis of heterogeneous catalysts in a multi-variable screening reactor

L29 ANSWER 6 OF 15 USPATFULL on STN; Methods and equipments of using dual functional catalyst of packing type

L29 ANSWER 7 OF 15 USPATFULL on STN; Dual functional catalyst of packing type and the catalytic distillation equipment

L29 ANSWER 8 OF 15 USPATFULL on STN; Process for preparing iodinated aromatic compounds

L29 ANSWER 9 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN; ORGANIC CHEMICAL OXIDATION DURING HYDROGEN PEROXIDE PRODUCTION; OXYDATION CHIMIQUE ORGANIQUE PENDANT LA PRODUCTION DE PEROXYDE D'HYDROGENE

L29 ANSWER 10 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN; PROCESS FOR EVAPORATION AND PROCESS VESSEL WITH INTEGRAL EVAPORATOR; PROCEDE D'EVAPORATION, ET RECIPIENT DE MISE EN OEUVRE A EVAPORATEUR INTEGRE

L29 ANSWER 11 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN; PROCESS FOR EVAPORATION IN AN ARRAY AND AN ARRAY OF PROCESS VESSELS WITH INTEGRAL EVAPORATOR; PROCEDE D'EVAPORATION DANS UN RESEAU ET RESEAU DE CUVES DE TRAITEMENT A EVAPORATEUR INTEGRE

L29 ANSWER 12 OF 15 PCTFULL COPYRIGHT 2004 Univentio on STN; METHODS FOR ANALYSIS OF HETEROGENEOUS CATALYSTS IN A MULTI-VARIABLE SCREENING REACTOR; ANALYSE DE CATALYSEURS HETEROGENES DANS UN REACTEUR DE CRIBLAGE MULTI-CRITERE

L29 ANSWER 13 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN; PRODUCTION OF OLEFINS.

L29 ANSWER 14 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN; PRODUCTION OF OLEFINS.

L29 ANSWER 15 OF 15 EUROPATFULL COPYRIGHT 2004 WILA on STN; PRODUCTION OF OLEFINS.

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L29 ANSWER 3 OF 15 USPATFULL on STN; Integrated hydrogen peroxide production and organic chemical oxidation

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